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## Author index to volume 291–300

- Abergel, D. and J.-Y. Lallemand, The stochastic Bloch equations driven by a coloured noise 298 (1998) 257
- Abreu, I., see Lima, J.C. 298 (1998) 189
- Abreu, P.E., see Varandas, A.J.C. 293 (1998) 261
- Achatz, U., S. Joos, C. Berg, M. Beyer, G. Niedner-Schatteburg and V.E. Bondybey, Generation of hydrated iodide clusters  $I^-(H_2O)_n$  by laser vaporization, their fragmentation and reactions with HCl 291 (1998) 459
- Achiba, Y., see Ishihara, S. 295 (1998) 475
- Achiwa, N., see Jamali, J.B. 292 (1998) 661
- Adachi, J., Y. Takata, N. Kosugi, E. Shigemasa, A. Yagishita and Y. Kitajima, Kinetic energy dependence of anisotropic yields of ionic fragmentations following S 1s excitations of  $SO_2$  294 (1998) 559
- Adamo, C. and V. Barone, Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model 298 (1998) 113
- Adamo, C., see Cossi, M. 297 (1998) 1
- Adamowicz, L., see Alexandrov, V. 291 (1998) 110
- Adamowicz, L., see Smets, J. 297 (1998) 451
- Adams, S.F. and T.A. Miller, Two-photon absorption laser-induced fluorescence of atomic nitrogen by an alternative excitation scheme 295 (1998) 305
- Adelt, M., S. Nepijko, W. Drachsel and H.-J. Freund, Size-dependent luminescence of small palladium particles 291 (1998) 425
- Agmon, N. and E.B. Krissinel, Incoherent control of protein conformational state 294 (1998) 79
- Agrawal, P.M., see Dabkara, N.K. 299 (1999) 125
- Agreiter, J., see Lorenz, M. 291 (1998) 291
- Ågren, H., see Minaev, B. 295 (1998) 455
- Ågren, H., see Norman, P. 296 (1998) 8
- Aguilar, A., see Huarte-Larrañaga, F. 291 (1998) 346
- Aguilar, A., see Romero, T. 292 (1998) 323
- Ahern, M.M., D.A. Steinhurst and M.A. Smith, Rotational relaxation of CO in He, Ar,  $N_2$  and CO free jets 300 (1999) 681
- Ahlborn, H., see Moore, P.B. 296 (1998) 259
- Ahlrichs, R., see Weigend, F. 294 (1998) 143
- Ahlskog, M., E. Seynaeve, R.J.M. Vullers, C. Van Haesendonck, A. Fonseca, K. Hernadi and J.B. Nagy, Ring formations from catalytically synthesized carbon nanotubes 300 (1999) 202
- Ahn, S. and W.S. Warren, Effects of intermolecular dipolar couplings in solution NMR in separated time intervals: the competition for coherence transfer pathways 291 (1998) 121
- Aida, M., H. Yamataka and M. Dupuis, Ab initio molecular dynamics simulations on the hydrolysis of methyl chloride with explicit consideration of three water molecules 292 (1998) 474

- Aida, M., see Yamataka, H. 300 (1999) 583  
Aigner, U., see Held, A. 299 (1999) 110  
Ajayan, P.M., see Banhart, F. 292 (1998) 554  
Aker, P.M., see Zhang, J.-X. 298 (1998) 183  
Akimoto, I., M. Ashida and K. Kan'no, Luminescence from  $C_{60}$  single crystals in glassy phase under site-selective excitation 292 (1998) 561  
Akimov, A.V., see Misochko, E.Ya. 293 (1998) 547  
Akiyama, K., see Sueki, K. 291 (1998) 37  
Akiyama, K., see Sueki, K. 300 (1999) 140  
Akkara, J.A., see Venugopal Rao, S. 297 (1998) 491  
Alacid, M., see Zúñiga, J. 298 (1998) 36  
Albertí, M., see Romero, T. 292 (1998) 323  
Albrecht, A.C., see Kirkwood, J.C. 293 (1998) 167  
Albrecht, A.C., see Kirkwood, J.C. 293 (1998) 417  
Albrecht, A.W., see Hybl, J.D. 297 (1998) 307  
Alcaraz, A., see Mafé, S. 294 (1998) 406  
Alexander, U.N., N.A. Trout, K.D. King and W.D. Lawrance, Phenylgermane as a suitable precursor for laser flash photolysis measurements of germylene kinetics 299 (1999) 291  
Alexandrov, V., S. Stepanian and L. Adamowicz, Theoretical ab initio study of O-H vibrational band in gas-phase glycine conformers 291 (1998) 110  
Ali, R., see Baig, M.A. 296 (1998) 403  
Alieva, E.V., L.A. Kuzik and V.A. Yakovlev, Sum frequency generation spectroscopy of thin organic films on silver using visible surface plasmon generation 292 (1998) 542  
Alikhani, M.E., see Krokidis, X. 292 (1998) 35  
Allègre, J., see Lamrabte, A. 295 (1998) 257  
Allen, M.D., T.C. Pesch, J.S. Robinson, A.J. Apponi, D.B. Grotjahn and L.M. Ziurys, The pure rotational spectrum of  $LiCH_3$  ( $\tilde{X}^1A$ ) 293 (1998) 397  
Alonso, J.A., see Gritsenko, O.V. 296 (1998) 307  
Alpert, B., see Haouz, A. 294 (1998) 197  
Alyea, E.C., see Wei, X. 300 (1999) 385  
Amaral, G., see Zhang, J. 299 (1999) 285  
Amat-Guerri, F., see Arbeloa, T.L. 299 (1999) 315  
Ambe, F., see Sueki, K. 300 (1999) 140  
Ambe, S., see Sueki, K. 300 (1999) 140  
Amler, E., see Konopasek, I. 293 (1998) 429  
Amor, N.B., see Pitarch-Ruiz, J. 291 (1998) 407  
Amos, R.D., see Van Caillie, C. 291 (1998) 71  
Amoureux, J.-P., see Pingel, U.-T. 294 (1998) 345  
Amutha, R., see Subramanian, V. 294 (1998) 285  
Anane, H., A. Jarid, A. Boutalib, I. Nebot-Gil and F. Tomás, Ab initio molecular orbital study of the substituent effect on phosphine-borane complexes 296 (1998) 277  
Andersen, K.B., see Møller, S. 291 (1998) 51  
Anderson, B.T., see Herbelin, J.M. 299 (1999) 583  
Anderson, D.T., see Krause, P.J. 294 (1998) 518  
Anderson, P.A., see Goldbach, A. 292 (1998) 137  
Anderson, S.M., J.I. Zink and D. Neuhauser, A simple and accurate approximation for a coupled system-bath: locally propagating gaussians 291 (1998) 387  
Andersson, M., see Holmgren, L. 296 (1998) 167

- Andrade, V., see Peric, M. 299 (1999) 69
- Andrejkovics, I. and Á. Nagy, Excitation energies in density functional theory: comparison of several methods for the H<sub>2</sub>O, N<sub>2</sub>, CO and C<sub>2</sub>H<sub>4</sub> molecules 296 (1998) 489
- Andreoni, W., see Curioni, A. 294 (1998) 263
- Andrés, J., see Oliva, M. 294 (1998) 87
- Andrés, J., see Sambrano, J.R. 294 (1998) 1
- Andrews, D.P., G.G. McFadyen and G.S. Beddard, Ultrafast electron transfer between methylene blue and liquid anilines 293 (1998) 343
- Andrievsky, G.V., V.K. Klochkov, E.L. Karyakina and N.O. Mchedlov-Petrosyan, Studies of aqueous colloidal solutions of fullerene C<sub>60</sub> by electron microscopy 300 (1999) 392
- Andriotis, A.N., M. Menon, G.E. Froudakis, Z. Fthenakis and J.E. Lowther, A tight-binding molecular dynamics study of Ni<sub>m</sub>Si<sub>n</sub> binary clusters 292 (1998) 487
- Anglaret, E., see Maser, W.K. 292 (1998) 587
- Ángyán, J.G., E. Rosta and P.R. Surján, Covalent bond orders and atomic valences from correlated wavefunctions 299 (1999) 1
- Anson, F.C., see Yu, H.Z. 293 (1998) 1
- Anupold, T., see Pingel, U.-T. 294 (1998) 345
- Anzai, H., see Nakatsuji, S. 296 (1998) 159
- Aogaki, R., see Nakabayashi, S. 294 (1998) 204
- Aoiz, F.J., M.T. Martínez, M. Menéndez, V. Sáez Rábanos and E. Verdasco, Quasiclassical trajectory study of the Li + HF(*v* = 0) → LiF + H reaction 299 (1999) 25
- Aoki, Y., see Yamazaki, T. 295 (1998) 431
- Apponi, A.J., M.A. Brewster and L.M. Ziurys, Rotational spectroscopy of LiCCH ( $\tilde{X} \Sigma$ ) in its ground and *v*<sub>5</sub> vibrational states 298 (1998) 161
- Apponi, A.J., see Allen, M.D. 293 (1998) 397
- Aquino, N., G. Campoy and H. Yee-Madeira, The inversion potential for NH<sub>3</sub> using a DFT approach 296 (1998) 111
- Aratono, Y., see Komaguchi, K. 300 (1999) 257
- Arbeloa, F.L., see Arbeloa, T.L. 299 (1999) 315
- Arbeloa, I.L., see Arbeloa, T.L. 299 (1999) 315
- Arbeloa, T.L., F.L. Arbeloa, I.L. Arbeloa, I. García-Moreno, A. Costela, R. Sastre and F. Amat-Guerri, Correlations between photophysics and lasing properties of dipyrromethene-BF<sub>2</sub> dyes in solution 299 (1999) 315
- Arcangeli, C., A.R. Bizzarri and S. Cannistraro, Role of interfacial water in the molecular dynamics-simulated dynamical transition of plastocyanin 291 (1998) 7
- Argollo de Menezes, M., see Gutterres, R.F. 300 (1999) 131
- Arkhipov, V.I., E.V. Emelianova and H. Bässler, Temperature-independent quantum yield of carrier photogeneration in weakly disordered conjugated polymers 296 (1998) 452
- Arnaud, R., V. Vetere and V. Barone, Regioselectivity of methyl radical addition to fluoroethenes: a quantum mechanical study 293 (1998) 295
- Arthur, N.L. and L.A. Miles, Rate constants for H + (CH<sub>3</sub>)<sub>4-n</sub>GeH<sub>n</sub>, *n* = 1-3 295 (1998) 531
- Asahi, T., see Hatanaka, K. 300 (1999) 727
- Asami, K., see Kometani, N. 294 (1998) 619
- Asano, T. and H. Sumi, An experimental examination of Biswas-Bagchi's prediction on the viscosity dependence of the rate of activated barrier surmounting in viscous liquids 294 (1998) 493
- Asaro, F., R. Gobetto, L. Liguori and G. Pellizer, Solution <sup>31</sup>P and <sup>59</sup>Co and solid-state <sup>31</sup>P CP/MAS NMR studies of triphenylphosphinecobaloximes 300 (1999) 414
- Aschenbrücker, J., see Ma, Y.-Z. 300 (1999) 465



- Ashida, M., see Akimoto, I. 292 (1998) 561
- Askar, A., see Dey, B.K. 297 (1998) 247
- Asmis, K.R., T.R. Taylor and D.M. Neumark, Anion photoelectron spectroscopy of  $\text{BN}^-$  295 (1998) 75
- Asmis, K.R., see Taylor, T.R. 297 (1998) 133
- Asmus, K.-D., see Brezová, V. 300 (1999) 667
- Assion, A., see Simon, M. 296 (1998) 579
- Asthana, B.P., see Singh, R.K. 296 (1998) 611
- Aubuchon, C.M., K.D. Rector, W. Holmes and M.D. Fayer, Nitro group asymmetric stretching mode lifetimes of molecules used in energetic materials 299 (1999) 84
- Avnir, D., see Keinan, S. 298 (1998) 43
- Avouris, P., see Rochefort, A. 297 (1998) 45
- Avron, J.E. and J. Berger, The Longuet-Higgins phase and charge transport in molecular rings 294 (1998) 13
- Awaga, K., T. Sekine, M. Okawa, W. Fujita, S.M. Holmes and G.S. Girolami, High-pressure effects on a manganese hexacyanomanganate ferrimagnet with  $T_N = 29\text{ K}$  293 (1998) 352
- Azamian, B.R., see Hafner, J.H. 296 (1998) 195
- Azria, R., see Le Coat, Y. 296 (1998) 208
- Ba, Y., C.I. Ratcliffe and J.A. Ripmeester, Quadrupolar echo double resonance (QEDOR) and solid echo double resonance (SOLEDOR) NMR 299 (1999) 201
- Bach, A. and S. Leutwyler, Water-chain clusters: vibronic spectra of 7-hydroxyquinoline  $\cdot (\text{H}_2\text{O})_n$ ,  $n = 1-4$  299 (1999) 381
- Bach, M., R. Georges, M. Hepp and M. Herman, Slit-jet Fourier transform infrared spectroscopy in  $^{12}\text{C}_2\text{H}_4$ : cold and hot bands near  $3000\text{ cm}^{-1}$  294 (1998) 533
- Bachels, T. and R. Schäfer, Formation enthalpies of Sn clusters: a calorimetric investigation 300 (1999) 177
- Bachilo, S., see Knyukshto, V. 297 (1998) 97
- Backov, R., see Lamrabte, A. 295 (1998) 257
- Bacskay, G.B., M. Martoprawiro and J.C. Mackie, The thermal decomposition of pyrrole: an ab initio quantum chemical study of the potential energy surface associated with the hydrogen cyanide plus propyne channel 300 (1999) 321
- Bacskay, G.B., see Schmidt, T.W. 292 (1998) 80
- Bae, C., see Lee, H.-S. 293 (1998) 97
- Baer, M., see Huarte-Larrañaga, F. 291 (1998) 346
- Bagryansky, V.A., V.I. Borovkov, Yu.N. Molin, M.P. Egorov and O.M. Nefedov, Quantum beats in the recombination fluorescence of radical ion pairs caused by the hyperfine coupling in radical anions 295 (1998) 230
- Bagus, P.S. and C. Wöll, Orientational effects in molecule-surface interactions: bonding directionality versus steric repulsion 294 (1998) 599
- Bai, C., see Zhou, S. 297 (1998) 77
- Baig, M.A., M. Yaseen, R. Ali, A. Nadeem and S.A. Bhatti, Near-threshold photoionization spectra of strontium 296 (1998) 403
- Bailey, W.C., B3LYP calculation of  $^{17}\text{O}$  quadrupole coupling constants in molecules 292 (1998) 71
- Bakker, B.L.G., D.H. Parker, G. Hancock and G.A.D. Ritchie, Two-photon dissociation of NO near 275 nm investigated by velocity map imaging 294 (1998) 565
- Bakker, M.P., see den Hartog, F.T.H. 297 (1998) 314
- Bakker, P., see Nagels, B. 294 (1998) 387
- Balasubramanian, K., see Feng, P.Y. 296 (1998) 283



- Balasubramanian, K., see Tan, H. 297 (1998) 173
- Baldelli, S., see Simonelli, D. 298 (1998) 400
- Bales, B.L., see Peric, M. 299 (1999) 69
- Balint-Kurti, G.G., see Meijer, A.J.H.M. 293 (1998) 270
- Ball, C.D. and F.C. De Lucia, Direct observation of  $\Lambda$ -doublet and hyperfine branching ratios for rotationally inelastic collisions of NO-He at 4.2 K 300 (1999) 227
- Balzer, F., S.D. Jett and H.-G. Rubahn, Alkali cluster films on insulating substrates: comparison between scanning force microscopy and extinction data 297 (1998) 273
- Bampos, N., see Thomas, P.J. 294 (1998) 229
- Baňacký, P., see Svrček, M. 299 (1999) 151
- Bando, Y., see Han, W. 299 (1999) 368
- Bandyopadhyay, S., Effect of variation of the size of  $\text{CH}_3$  and  $\text{CH}_2$  groups on cage-to-cage migration of *n*-butane in zeolite NaCaA 293 (1998) 378
- Banhart, F., Ph. Redlich and P.M. Ajayan, The migration of metal atoms through carbon onions 292 (1998) 554
- Baranov, L.Ya., A. Held, H.L. Selzle and E.W. Schlag, Long lived Rydberg ZEKE states using fast programmed electric pulses. I. The basic method 291 (1998) 311
- Baranov, L.Ya., see Held, A. 291 (1998) 318
- Baranov, L.Ya., see Held, A. 299 (1999) 110
- Barborini, E., P. Piseri, A. Li Bassi, A.C. Ferrari, C.E. Bottani and P. Milani, Synthesis of carbon films with controlled nanostructure by separation of neutral clusters in supersonic beams 300 (1999) 633
- Barbosa, M.C., see Kuhn, P.S. 298 (1998) 51
- Barford, W., see Bursill, R.J. 294 (1998) 305
- Bargon, J., see Natterer, J. 293 (1998) 455
- Barjat, H., see Linden, N. 296 (1998) 61
- Barker, P.D., see Goldbach, A. 292 (1998) 137
- Barnes, M.D., see Runge, K. 299 (1999) 352
- Baronavski, A.P., see Owrutsky, J.C. 293 (1998) 555
- Barone, V., see Adamo, C. 298 (1998) 113
- Barone, V., see Arnaud, R. 293 (1998) 295
- Barone, V., see Cossi, M. 297 (1998) 1
- Barone, V., see Rega, N. 293 (1998) 221
- Barrow, M.P., N.J. Tower, R. Taylor and T. Drewello, Matrix-assisted laser-induced gas-phase aggregation of  $\text{C}_{60}$  oxides 293 (1998) 302
- Bartels, L., G. Meyer and K.-H. Rieder, High-resolution spectroscopy of weakly chemisorbed species using a low-temperature scanning tunneling microscope (STM): CO/Cu(111) 297 (1998) 287
- Bartels, L., M. Wolf, G. Meyer and K.-H. Rieder, On the diffusion of 'hot' adsorbates: a non-monotonic distribution of single particle diffusion lengths for CO/Cu(111) 291 (1998) 573
- Barth, H.-D., see Hobza, P. 299 (1999) 180
- Bartkowiak, W. and J. Lipiński, Finite-field calculations of the second-order hyperpolarizabilities  $\gamma$  of molecules in solutions 292 (1998) 92
- Bartl, A., see Kuran, P. 292 (1998) 580
- Bartlett, R.J., see Gutsev, G.L. 291 (1998) 547
- Bartlett, R.J., see Gutsev, G.L. 292 (1998) 289
- Basch, H. and S. Hoz, Resonance in formamide: resolution of contending models 294 (1998) 117
- Baskin, J.S., see Yu, H.Z. 293 (1998) 1

- Bässler, H., see Arkhipov, V.I. 296 (1998) 452
- Bastida, A., see Zúñiga, J. 298 (1998) 36
- Basu Kumar, A., N. Vaval and S. Pal, An extended coupled-cluster functional for molecular properties: study of an analytical and numerical approach 295 (1998) 189
- Bataiev, M.M., see Scheblykin, I.G. 298 (1998) 341
- Bauer, F., see Pingel, U.-T. 294 (1998) 345
- Baumgärtel, H., see Boyle, K.J. 294 (1998) 507
- Bauschlicher Jr., C.W. and H. Partridge, The atomization energy of  $Mg_4$  300 (1999) 364
- Bazan, G.C., see Khan, M.I. 298 (1998) 309
- Bearpark, M.J., see Klein, S. 292 (1998) 259
- Beck, C., see Hauschildt, J. 300 (1999) 569
- Becker, I., see Kim, J. 297 (1998) 90
- Becker, J.A., see Hihara, T. 294 (1998) 357
- Becker, K.H., C. Dinis, H. Geiger and P. Wiesen, Kinetics of the reaction of OH with di-*n*-butoxymethane (DBM) in the range 298–710 K 300 (1999) 460
- Beddard, G.S., see Andrews, D.P. 293 (1998) 343
- Belchior, J.C., see Lemes, N.H.T. 296 (1998) 233
- Beljonne, D., see Kogej, T. 298 (1998) 1
- Belletête, M., see DiCésare, N. 291 (1998) 487
- Belletête, M., see Shen, X. 298 (1998) 201
- Bello, I., see Wang, N. 299 (1999) 237
- Ben-Nun, M. and T.J. Martínez, Ab initio molecular dynamics study of *cis-trans* photoisomerization in ethylene 298 (1998) 57
- Benito, A.M., see Maser, W.K. 292 (1998) 587
- Bennett, M.A., see Gopinath, C.S. 296 (1998) 566
- Berard, D.R., see Pavese, M. 300 (1999) 93
- Berardi, R., C. Fava and C. Zannoni, A Gay-Berne potential for dissimilar biaxial particles 297 (1998) 8
- Berardi, R., see Stelzer, J. 299 (1999) 9
- Berberan-Santos, M.N., see Bodunov, E.N. 297 (1998) 419
- Berdinsky, V.L., see Buchachenko, A.L. 298 (1998) 279
- Berg, A., see Shuali, Z. 300 (1999) 687
- Berg, C., see Achatz, U. 291 (1998) 459
- Berger, J., see Avron, J.E. 294 (1998) 13
- Berger, R., H.P. Lang, Ch. Gerber, J.K. Gimzewski, J.H. Fabian, L. Scandella, E. Meyer and H.-J. Güntherodt, Micromechanical thermogravimetry 294 (1998) 363
- Berlin, Y.A. and L.D.A. Siebbeles, Energy relaxation during thermally activated diffusion along one-dimensional chains with site disorder 291 (1998) 85
- Bernardi, F., see Klein, S. 292 (1998) 259
- Bernath, P., M. Carleer, S. Fally, A. Jenouvrier, A.C. Vandaele, C. Hermans, M.-F. Mérienne and R. Colin, The Wulf bands of oxygen 297 (1998) 293
- Bernhardt, T.M., see Zhong, D. 298 (1998) 129
- Bernholc, J., see Buongiorno Nardelli, M. 296 (1998) 471
- Bernier, P., see Kuhlmann, U. 294 (1998) 237
- Berning, A., see Hübner, O. 294 (1998) 37
- Bernshtein, V. and I. Oref, Energy release in benzene-argon cluster dissociation – quasiclassical trajectory calculations 300 (1999) 104
- Berovic, N., see Thomas, P.J. 294 (1998) 229
- Bersohn, R., see Min, Z. 296 (1998) 372

- Bertmer, M., see Chan, J.C.C. 292 (1998) 154
- Besenbacher, F., see Pedersen, M.Ø. 299 (1999) 403
- Beyer, M., see Achatz, U. 291 (1998) 459
- Bezel, I., see Liu, K. 299 (1999) 374
- Bhattacharyya, S., L.R. Sousa and S. Ghosh, Study of energy transfer in a naphthalene-linked crown ether-Eu<sup>3+</sup> complex: the effect of the orientation of the naphthalene  $\pi$ -plane with respect to the Eu<sup>3+</sup> ion 297 (1998) 154
- Bhattacharyya, S.P., see Chaudhury, P. 296 (1998) 51
- Bhatti, S.A., see Baig, M.A. 296 (1998) 403
- Bhriuvansh, P., see Singh, R.K. 296 (1998) 611
- Bianco, A., see Casaboni, M. 291 (1998) 167
- Bieske, E.J., see Weiser, P.S. 299 (1999) 303
- Bievetski, A., see Meier, R. 292 (1998) 507
- Bifone, A., see La Penna, G. 294 (1998) 447
- Bifone, A., see Wolber, J. 296 (1998) 391
- Bilger, C. and B. Pettinger, The SHG anisotropy pattern of a reconstructed gold(110) electrode 294 (1998) 425
- Billing, G.D. and A. Kuppermann, On the geometric phase effect on tetra-atomic reactions: the OH + H<sub>2</sub> → H<sub>2</sub>O + H reaction 294 (1998) 26
- Binnemans, K., R. Van Deun, D.W. Bruce and Yu.G. Galyametdinov, Influence of the lanthanide contraction on the transition temperatures of rare-earth containing metallomesogens with Schiff base ligands 300 (1999) 509
- Birch, D.J.S., see Volkmer, A. 299 (1999) 395
- Biskupič, S., see Bittererová, M. 299 (1999) 145
- Biskupič, S., see Svrček, M. 299 (1999) 151
- Biswas, N. and S. Umapathy, Partitioning of the total reorganization energy into its vibrational and solvent (inertial and reorientational) contributions using resonance Raman intensities 294 (1998) 181
- Bittererová, M. and S. Biskupič, Ab initio calculation of stationary points on the HF<sub>2</sub> potential energy surface 299 (1999) 145
- Bittl, R., see Jeschke, G. 294 (1998) 323
- Bizzarri, A.R., see Arcangeli, C. 291 (1998) 7
- Bizzocchi, L., C. Degli Esposti and F. Tamassia, Detection of perturbation-allowed  $\Delta J = 2$  transitions in the millimetre-wave spectrum of <sup>81</sup>BrNO 293 (1998) 441
- Bjørnstad, A., see Ruoff, P. 291 (1998) 249
- Blomberg, M.R.A., see Siegbahn, P.E.M. 292 (1998) 421
- Bloor, D., Dissolution and thermochromism of polydiacetylenes with chiral pendent groups 295 (1998) 63
- Bocanegra, J.M., see Romero, T. 292 (1998) 323
- Bocquet, M.-L., see Pedersen, M.Ø. 299 (1999) 403
- Bodunov, E.N., M.N. Berberan-Santos and J.M.G. Martinho, Electronic energy transfer between molecules diffusing on spherical particles: approximate expressions for the decay law of the donor 297 (1998) 419
- Boelens, R., see Karimi-Nejad, Y. 300 (1999) 706
- Boero, M., see Curioni, A. 294 (1998) 263
- Boese, A.D. and G.E. Scuseria, C<sub>2</sub> fragmentation energy of C<sub>60</sub> revisited: theory disagrees with most experiments 294 (1998) 233
- Böhm, M.C., see Ramírez, R. 291 (1998) 44
- Boissel, P., see Gee, C. 298 (1998) 85



- Bonadeo, H., see Burgos, E. 298 (1998) 273
- Bonadeo, H., see Halac, E. 299 (1999) 64
- Bondybey, V.E., see Achatz, U. 291 (1998) 459
- Bondybey, V.E., see Kraus, D. 295 (1998) 285
- Bondybey, V.E., see Lorenz, M. 291 (1998) 291
- Bonetti, M., see Oleinikova, A. 299 (1999) 417
- Bonnet, L. and J.C. Rayez, Statistical analysis of the recoil energy distributions in the products of the unimolecular dissociations of  $\text{NO}_2$  and  $\text{C}_2\text{O}$  296 (1998) 19
- Booij, A.S., see Konings, R.J.M. 292 (1998) 447
- Boon, G., F. De Proft, W. Langenaeker and P. Geerlings, The use of density functional theory-based reactivity descriptors in molecular similarity calculations 295 (1998) 122
- Bordat, P. and R. Brown, Correspondence between electronic origins and substitution sites in pentacene/*p*-terphenyl mixed crystals by molecular modelling 291 (1998) 153
- Borin, I.A. and M.S. Skaf, Molecular association between water and dimethyl sulfoxide in solution: the librational dynamics of water 296 (1998) 125
- Borovkov, V.I., see Bagryansky, V.A. 295 (1998) 230
- Borovykh, I.V., see Proskuryakov, I.I. 299 (1999) 566
- Borowicz, P., A. Grabowska, A. Leś, Ł. Kaczmarek and B. Zagrodzki, New phototautomerizing systems: non-symmetric derivatives of [2,2'-bipyridyl]-3,3'-diol 291 (1998) 351
- Borzsák, I. and P.T. Cummings, Molecular dynamics simulation of ice XII 300 (1999) 359
- Bosanac, S.D. and J.N. Murrell, Unimolecular dissociation dynamics of helium cluster ions 291 (1998) 64
- Bottani, C.E., see Barborini, E. 300 (1999) 633
- Bouas-Laurent, H., see Zehnacker, A. 293 (1998) 357
- Bouhedja, Y., see Ksenofontov, V. 294 (1998) 545
- Boutalib, A., see Anane, H. 296 (1998) 277
- Bowen, J.P., see Kirschner, K.N. 295 (1998) 204
- Bowers, M.T., see Kemper, P.R. 293 (1998) 503
- Bowman, R.M., see Prater, K. 295 (1998) 82
- Bowron, D.T., A. Filipponi, C. Lobban and J.L. Finney, Temperature-induced disordering of the hydrophobic hydration shell of Kr and Xe 293 (1998) 33
- Boyle, K.J., D.P. Secombe, R.P. Tuckett, H. Baumgärtel and H.W. Jochims, Vacuum-UV fluorescence spectroscopy of  $\text{GeF}_4$  in the 10-25 eV range 294 (1998) 507
- Bradforth, S.E., see Klopfer, J.A. 298 (1998) 120
- Braga, J.P., see Lemes, N.H.T. 296 (1998) 233
- Brahimi, M., see Del Re, G. 299 (1999) 511
- Brakenhoff, G.J., see van Oijen, A.M. 292 (1998) 183
- Branca, M., see Rustici, M. 293 (1998) 145
- Bratcher, M.S., see Grunnet-Jepsen, A. 291 (1998) 553
- Bratos, S. and J.-Cl. Leicknam, Pump-probe absorption anisotropy of the hydrated electron. A theory 291 (1998) 496
- Braun, M., see Herwig, A. 300 (1999) 269
- Brédas, J.L., see Kogej, T. 298 (1998) 1
- Brede, O., see Häupl, T. 291 (1998) 215
- Brewster, M.A., see Apponi, A.J. 298 (1998) 161
- Brezová, V., A. Staško, D. Dvoranová, K.-D. Asmus and D.M. Guldi, Photochemical reduction of  $\text{C}_{60}$  derivatives in aqueous systems containing titanium dioxide or ascorbic acid (EPR study) 300 (1999) 667
- Brion, C.E., see Pang, W.N. 299 (1999) 207



- Brocklehurst, B., see Till, U. 298 (1998) 7
- Broitman, E., see Suenaga, K. 300 (1999) 695
- Bronikowski, M.J., see Hafner, J.H. 296 (1998) 195
- Bronsveld, M.V., X.L.R. Dauw and E.J.J. Groenen, The triplet state of  $C_{70}$ . A zero-field study 293 (1998) 528
- Bröring, M., see Shuali, Z. 300 (1999) 687
- Broude, S., J.O. Jung and R.B. Gerber, Combined diffusion quantum Monte Carlo-vibrational self-consistent field (DQMC-VSCF) method for excited vibrational states of large polyatomic systems 299 (1999) 437
- Brouillard, R., see Lima, J.C. 298 (1998) 189
- Brown, F.L.H. and R.J. Silbey, Quantum control for arbitrary linear and quadratic potentials 292 (1998) 357
- Brown, M.G., see Cruzan, J.D. 292 (1998) 667
- Brown, R., see Bordat, P. 291 (1998) 153
- Brown, S.S., R.K. Talukdar and A.R. Ravishankara, Rate constants for the reaction  $OH + NO_2 + M \rightarrow HNO_3 + M$  under atmospheric conditions 299 (1999) 277
- Brown, W.A., Q. Ge, R.K. Sharma and D.A. King, Lateral potential energy surfaces for molecular chemisorption on metals from experiment and theory: NO on Pt{110}-(1  $\times$  2) 299 (1999) 253
- Brown, W.A., see Sharma, R.K. 291 (1998) 1
- Bruce, D.W., see Binnemans, K. 300 (1999) 509
- Brunetti, A., see Rustici, M. 293 (1998) 145
- Brunetti, B., P. Candori, R. Ferramosche, S. Falcinelli, F. Vecchiocattivi, A. Sassara and M. Chergui, Penning ionization of  $C_{60}$  molecules 294 (1998) 584
- Brüning, F., S. Matejcik, E. Illenberger, Y. Chu, G. Senn, D. Muigg, G. Denifl and T.D. Märk, Effects of temperature on the dissociative electron attachment to  $N_2O$  292 (1998) 177
- Brunner, E., see Haake, M. 292 (1998) 686
- Brüschweiler, R., see Fel'dman, E.B. 294 (1998) 297
- Brutschy, B., see Hobza, P. 299 (1999) 180
- Brutschy, B., see Riehn, C. 299 (1999) 103
- Buchachenko, A.A., Predissociation of the  $Rg \cdots I_2(B)$  ( $Rg = Ne, Ar, Kr$ ) complexes: simulations based on the first-order diatomics-in-molecule perturbation theory 292 (1998) 273
- Buchachenko, A.L. and V.L. Berdinsky, Spin catalysis as a nuclear spin selective process 298 (1998) 279
- Bucher, C.R. and K.K. Lehmann, Vibrationally mediated photodissociation of HCN 294 (1998) 173
- Buchhold, K., see Hobza, P. 299 (1999) 180
- Buckingham, A.D. and P. Fischer, Linear electro-optic effect in optically active liquids 297 (1998) 239
- Buczowski, M., see Fisz, J.J. 296 (1998) 34
- Buda, F., see La Penna, G. 294 (1998) 447
- Bulcock, S., see Chen, Y. 299 (1999) 260
- Bulthuis, J., see de Lange, M.J.L. 294 (1998) 332
- Buongiorno Nardelli, M., C. Roland and J. Bernholc, Theoretical bounds for multiwalled carbon nanotube growth 296 (1998) 471
- Burget, D. and P. Jacques, Unusual solvent effects on the fluorescence quenching rate constants of a thioxanthone derivative by *n*-butylamine and isoprene 291 (1998) 207
- Burgos, E., E. Halac and H. Bonadeo, A semi-empirical potential for the statics and dynamics of covalent carbon systems 298 (1998) 273
- Burgos, E., see Halac, E. 299 (1999) 64
- Burrows, B.L. and M. Cohen, Accurate approximate analytical solutions for a double-well potential 295 (1998) 389

- Bursill, R.J., C. Castleton and W. Barford, Optimal parametrisation of the Pariser-Parr-Pople Model for benzene and biphenyl 294 (1998) 305
- Cabaleiro-Lago, E.M. and M.A. Ríos, A cooperative mechanism as the main source of the marked structural differences between solid and gaseous  $\text{HCN} \cdots \text{BF}_3$  294 (1998) 272
- Cabaleiro-Lago, E.M. and M.A. Ríos, Erratum to "A cooperative mechanism as the main source of the marked structural differences between solid and gaseous  $\text{HCN} \cdots \text{BF}_3$ . [Chem. Phys. Lett. 294 (1998) 272]" 299 (1999) 358
- Cai, Z.-L. and J.P. François, Ab initio study of the lowest  $^3\Sigma^-$ ,  $^3\Pi$  and  $^1\Sigma^+$  states of the  $\text{SiN}^+$  cation 300 (1999) 69
- Calaminici, P., see Martínez, A. 299 (1999) 630
- Calucci, L., M. Geppi, C.A. Veracini and R.Y. Dong, Molecular rotation and conformational transitions studied by  $^2\text{H}$  NMR in a smectogen 296 (1998) 357
- Calvo, F., Free-energy calculation for rotating systems using the Monte Carlo method 291 (1998) 393
- Calvo, F., see Zhang, F.S. 300 (1999) 595
- Caminati, W., S. Melandri, A. Millemaggi and P.G. Favero, Rotational spectrum of the imidazole-argon complex 294 (1998) 377
- Campargue, A., see Garnache, A. 292 (1998) 698
- Campbell, M.L., Kinetic study of gas-phase  $\text{Y}(\text{a}^2\text{D}_{3/2})$  and  $\text{La}(\text{a}^2\text{D}_{3/2})$  with  $\text{O}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{CO}_2$  and  $\text{NO}$  294 (1998) 339
- Campoy, G., see Aquino, N. 296 (1998) 111
- Candori, P., see Brunetti, B. 294 (1998) 584
- Cannistraro, S., see Arcangeli, C. 291 (1998) 7
- Canpolat, M., F.W. Starr, A. Scala, M.R. Sadr-Lahijany, O. Mishima, S. Havlin and H.E. Stanley, Local structural heterogeneities in liquid water under pressure 294 (1998) 9
- Cao, G., Y. Seimiya, Y. Ohno and T. Matsushima, Reaction sites working in steady-state CO oxidation on a stepped Pt(113) surface 294 (1998) 419
- Cao, H., see Gao, X.-C. 297 (1998) 530
- Cao, X., X. Qian, C. Qiao and D. Wang, A kinetic study of the isomerization reaction from  $\text{SSF}_2$  to  $\text{FSSF}$  using the HeI photoelectron spectroscopic method 299 (1999) 322
- Capellini, G., see Polzonetti, G. 292 (1998) 515
- Cappelletti, R.L., see Guerrero, H.M. 297 (1998) 265
- Caragiu, M., see Seyller, Th. 291 (1998) 567
- Caravati, C., see Rustici, M. 293 (1998) 145
- Carleer, M., see Bernath, P. 297 (1998) 293
- Carrick, P.G., see Presilla-Márquez, J.D. 300 (1999) 719
- Carrington Jr., T., see Chakrabarti, N. 293 (1998) 209
- Carter, E.A., see Govind, N. 295 (1998) 129
- Cartier, A., see Salvatella, L. 296 (1998) 239
- Casalboni, M., F. De Matteis, V. Ferone, P. Proposito, R. Senesi, R. Pizzoferrato, A. Bianco and A. De Mico, DODCI molecules incorporated in sol-gel glasses: the interaction with the silica matrix 291 (1998) 167
- Casarin, M., C. Maccato and A. Vittadini, A comparative study of the  $\text{NH}_3$  chemisorption on  $\text{ZnO}(10\bar{1}0)$  and  $\text{Cu}_2\text{O}(111)$  non-polar surfaces 300 (1999) 403
- Caspary, N., see Lorenz, M. 291 (1998) 291
- Cassell, A.M., see Kong, J. 292 (1998) 567
- Cassidei, L., see Petrella, G. 291 (1998) 562
- Castell Marcos, O., see Pérez-Casany, M.P. 295 (1998) 181

- Castleton, C., see Bursill, R.J. 294 (1998) 305
- Catalán, J., On the first triplet state of benzotriazole-like ultraviolet stabilizers 297 (1998) 549
- Catalán, J. and J. Palomar, Gas-phase protolysis between a neutral Brønsted acid and a neutral Brønsted base? 293 (1998) 511
- Cavell, R.G., see Neville, J.J. 300 (1999) 451
- Cazzoli, G., see Dore, L. 300 (1999) 489
- Cederbaum, L.S., see Worth, G.A. 299 (1999) 451
- Cerasari, S., see Kelling, S. 293 (1998) 325
- Chabalowski, C.F., see Manaa, M.R. 300 (1999) 619
- Chachisvilis, M., I. Garcia-Ochoa, A. Douhal and A.H. Zewail, Femtochemistry in nanocavities: dissociation, recombination and vibrational cooling of iodine in cyclodextrin 293 (1998) 153
- Chakrabarti, N., T. Carrington Jr. and B. Roux, Rate constants in quantum mechanical systems: A rigorous and practical path-integral formulation for computer simulations 293 (1998) 209
- Chakraborty, D. and S. Manogaran, Vibrational analysis of glycine zwitterion – an ab initio study 294 (1998) 56
- Chan, I.Y., see Schenker, S. 297 (1998) 281
- Chan, J.C.C., M. Bertmer and H. Eckert, Double-quantum cross-polarization between half-integer quadrupolar spin systems:  $^{11}\text{B} \leftrightarrow ^{23}\text{Na}$  and  $^{11}\text{B} \leftrightarrow ^{27}\text{Al}$  292 (1998) 154
- Chan, W.-T. and I.P. Hamilton, Geometries and vibrational frequencies for calcium and strontium radical salts of H, F, Cl, Br, I, OH, SH, CN, NC, CCH, NNN, NCO, NCS,  $\text{NH}_2$ ,  $\text{CH}_3$ ,  $\text{OCH}_3$ ,  $\text{SCH}_3$ ,  $\text{HCOO}$ ,  $\text{CH}_3\text{COO}$ ,  $\text{HCONH}$  and  $\text{HCONCH}_3$  297 (1998) 217
- Chan, W.-T. and I.P. Hamilton, Improved potential function for  $\text{HOO}^-/\text{OOH}^-$  isomerization 292 (1998) 57
- Chandra, P., see Malkina, O.L. 296 (1998) 93
- Chang, B.H., see Pan, Z.W. 299 (1999) 97
- Chapovsky, P.L., see Il'ichov, L.V. 297 (1998) 439
- Chapovsky, P.L., see Nagels, B. 294 (1998) 387
- Chattopadhyay, S., see Mohan, H. 300 (1999) 493
- Chaturvedi, S., see Rodriguez, J.A. 296 (1998) 421
- Chaudhuri, P., see Das, U.K. 298 (1998) 211
- Chaudhury, P. and S.P. Bhattacharyya, Numerical solutions of the Schrödinger equation directly or perturbatively by a genetic algorithm: test cases 296 (1998) 51
- Chazalviel, J.-N., see Maroun, F. 292 (1998) 493
- Cheetham, A.K., see Satishkumar, B.C. 300 (1999) 473
- Chemerisov, S.D., D.W. Werst and A.D. Trifunac, Electron spin relaxation and rotational dynamics of tetramethylethylene radical cation in ZSM5 291 (1998) 262
- Chen, B., see Curotto, E. 295 (1998) 366
- Chen, C., see Zhang, T. 298 (1998) 236
- Chen, E.C.M. and E.S. Chen, Characterization of homonuclear diatomic ions by semi-empirical Morse potential energy curves. 3. Rare-gas positive ions revisited 293 (1998) 491
- Chen, E.S., see Chen, E.C.M. 293 (1998) 491
- Chen, G.H., see Yokojima, S. 292 (1998) 379
- Chen, G.H., see Yokojima, S. 300 (1999) 540
- Chen, J., see Chen, Y. 299 (1999) 532
- Chen, J.M., R.S. Liu, M.J. Kramer, K.W. Dennis and R.W. McCallum, Soft X-ray absorption study of  $(\text{Nd}_{1.05-x}\text{Pr}_x)\text{Ba}_{1.95}\text{Cu}_3\text{O}_7$  using synchrotron radiation 294 (1998) 209
- Chen, X.H., see He, R.R. 298 (1998) 170



- Chen, X.J., see Pang, W.N. 296 (1998) 605
- Chen, X.J., see Pang, W.N. 299 (1999) 207
- Chen, Y., J. Chen, H. Hu, M.A. Hamon, M.E. Itkis and R.C. Haddon, Solution-phase EPR studies of single-walled carbon nanotubes 299 (1999) 532
- Chen, Y., J. Fitz Gerald, J.S. Williams and S. Bulcock, Synthesis of boron nitride nanotubes at low temperatures using reactive ball milling 299 (1999) 260
- Chen, Y., see Pryor, B.A. 299 (1999) 536
- Chen, Y.-C., see Chou, P.-T. 294 (1998) 579
- Chen, Y.-C., see Chou, P.-T. 299 (1999) 327
- Cheng, Y.F., see Zheng, X. 292 (1998) 295
- Cherepkov, N.A., see Semenov, S.K. 291 (1998) 375
- Chergui, M., see Brunetti, B. 294 (1998) 584
- Chergui, M., see Portella-Oberli, M.T. 296 (1998) 323
- Chergui, M., see Vigliotti, F. 296 (1998) 316
- Chernozatonskii, L.A., Polymerized nanotube structures – new zeolites? 297 (1998) 257
- Chernyak, V., see Tretiak, S. 297 (1998) 357
- Cheshnovsky, O., see Kim, J. 297 (1998) 90
- Cheung, A.S.-C., see He, J. 295 (1998) 535
- Cho, W.R., see Kang, H. 292 (1998) 213
- Choe, Y.-K., T. Hashimoto, H. Nakano and K. Hirao, Theoretical study of the electronic ground state of iron(II) porphine 295 (1998) 380
- Choho, K., see Safi, B. 300 (1999) 85
- Choi, L.-S., see Clays, K. 293 (1998) 337
- Choi, Y.S., see Yoon, M.-C. 300 (1999) 207
- Chong, S.-H. and F. Hirata, Effect of molecular symmetry on electrical potential fluctuations of solvent around solute in polar liquid 293 (1998) 119
- Chou, P.-T., Y.-C. Chen and C.-Y. Wei, Photophysical properties of  $(O_2(^1\Delta_g))_2$  in solution phase 294 (1998) 579
- Chou, P.-T., Y.-C. Chen, W.-S. Yu, M.-Z. Lee and C.-Y. Wei, Photodissociation of  $I_2$  in solution: the observation of solvent-dependent near-infrared emission associated with  $I(^2P_{1/2})$ -solvent interaction 299 (1999) 327
- Christiansen, O., J. Gauss and J.F. Stanton, The effect of triple excitations in coupled cluster calculations of frequency-dependent polarizabilities 292 (1998) 437
- Christiansen, O., see Gauss, J. 296 (1998) 117
- Chu, S.-I. and X.-M. Tong, Time-dependent approach to high-resolution spectroscopy: application to the photoabsorption spectrum of classically chaotic hydrogen atoms in magnetic fields 294 (1998) 31
- Chu, S.-Y., see Su, M.-D. 298 (1998) 107
- Chu, Y., see Brüning, F. 292 (1998) 177
- Ciriaco, F., see Petrella, G. 291 (1998) 562
- Cirujeda, J., see García-Muñoz, J.L. 293 (1998) 160
- Civalleri, B., C.M. Zicovich-Wilson, P. Ugliengo, V.R. Saunders and R. Dovesi, A periodic ab initio study of the structure and relative stability of silica polymorphs 292 (1998) 394
- Civalleri, B., E. Garrone and P. Ugliengo, Cage-like clusters as models for the hydroxyls of silica: ab initio calculation of  $^1H$  and  $^{29}Si$  NMR chemical shifts 299 (1999) 443
- Civalleri, B., E. Garrone and P. Ugliengo, Vibrational modes of isolated hydroxyls of silica computed ab initio in a cluster approach 294 (1998) 103
- Clark, C.D., see Hynes, A.J. 295 (1998) 25

- Clary, D.C., see Krause, P.J. 294 (1998) 518
- Claus, R.O., see Liu, Y. 298 (1998) 315
- Clays, K., G. Olbrechts, T. Munters, A. Persoons, O.-K. Kim and L.-S. Choi, Enhancement of the molecular hyperpolarizability by a supramolecular amylose–dye inclusion complex, studied by hyper-Rayleigh scattering with fluorescence suppression 293 (1998) 337
- Cocco, D., see Polzonetti, G. 292 (1998) 515
- Cohen, A.J. and Y. Tantirungrotechai, Molecular electric properties: an assessment of recently developed functionals 299 (1999) 465
- Cohen, M., see Burrows, B.L. 295 (1998) 389
- Colbert, D.T., see Hafner, J.H. 296 (1998) 195
- Colic, M. and M.L. Fisher, Effect of the size and affinity for water of excluded ions on interparticle forces 291 (1998) 24
- Colin, R., see Bernath, P. 297 (1998) 293
- Collier, C.P., see Remacle, F. 291 (1998) 453
- Colliex, C., see Suenaga, K. 300 (1999) 695
- Comes, F.J., see Pfeiffer, T. 298 (1998) 351
- Čomor, M.I. and J.M. Nedeljković, Room-temperature luminescence of AgBr quantum dots 299 (1999) 233
- Compagnini, G., see Pignataro, B. 299 (1999) 430
- Consalvo, C., see Pignataro, B. 299 (1999) 430
- Consalvo, D. and U. Spoerel, The electric dipole moment of tetrahydropyran–water 297 (1998) 543
- Contreras, R., see Pérez, P. 293 (1998) 239
- Cooke, S.A., G.K. Corlett and A.C. Legon, Comparisons of the interactions of benzene, furan and thiophene with Lewis acids: the rotational spectrum of thiophene ··· HF 291 (1998) 269
- Cooke, S.A., J.H. Holloway and A.C. Legon, Rotational spectrum of thiophene ··· ClF and the role of thiophene as a  $\pi$ - or  $n$ -electron pair donor in weakly bound complexes 298 (1998) 151
- Coonan, M.H. and G.L.D. Ritchie, Cotton–Mouton effect and optical-frequency molecular polarizability anisotropy of ethylene 293 (1998) 197
- Cordero, N.A., see Gritsenko, O.V. 296 (1998) 307
- Coriani, S., C. Hättig, P. Jørgensen, A. Halkier and A. Rizzo, Erratum to: “Coupled cluster calculations of Verdet constants”. [Chem. Phys. Lett. 281 (1997) 445] 293 (1998) 324
- Coriani, S., P. Jørgensen, A. Rizzo, K. Ruud and J. Olsen, Ab initio determinations of magnetic circular dichroism 300 (1999) 61
- Coriani, S., see Halkier, A. 294 (1998) 292
- Corlett, G.K., see Cooke, S.A. 291 (1998) 269
- Cossi, M., C. Adamo and V. Barone, Solvent effects on an  $S_N2$  reaction profile 297 (1998) 1
- Cossi, M., see Rega, N. 293 (1998) 221
- Costa, C., see Magnasco, V. 291 (1998) 529
- Costa, D., F. Saija and P.V. Giaquinta, Erratum to: “Angular correlations and statistical entropy of hard spherocylinders: the isotropic–nematic transition”. [Chem. Phys. Lett. 283 (1998) 86–90] 291 (1998) 252
- Costa, D., F. Saija and P.V. Giaquinta, Erratum to: “Angular correlations and statistical entropy of hard spherocylinders: the isotropic–nematic transition”. [Chem. Phys. Lett. 283 (1998) 86–90] 299 (1999) 252
- Costela, A., see Arbeloa, T.L. 299 (1999) 315
- Cox, S.F.J., see García-Muñoz, J.L. 293 (1998) 160
- Cremer, D., E. Kraka and P.G. Szalay, Decomposition modes of dioxirane, methyldioxirane and dimethyldioxirane — a CCSD(T), MR-AQCC and DFT investigation 292 (1998) 97
- Creve, S., see Nguyen, M.T. 293 (1998) 90

- Crippa, P.R., see Murgida, D.H. 294 (1998) 538
- Cruz, D.A. and M. Xiao, Atom-surface interaction potential for  $^4\text{He}$ -NaCl(001) system: a modified pairwise close-coupling calculation 297 (1998) 225
- Cruzan, J.D., M.R. Viant, M.G. Brown, D.D. Lucas, K. Liu and R.J. Saykally, Terahertz laser vibration-rotation-tunneling spectrum of the water pentamer- $\text{d}_{10}$ . Constraints on the bifurcation tunneling dynamics 292 (1998) 667
- Császár, A.G., J.S. Kain, O.L. Polyansky, N.F. Zobov and J. Tennyson, Relativistic correction to the potential energy surface and vibration-rotation levels of water 293 (1998) 317
- Cukrowski, A.S. and M.A. Telka, The role of nonequilibrium effects on negative Arrhenius activation energy in a Lorentz gas 297 (1998) 402
- Cummings, P.T., see Borzsák, I. 300 (1999) 359
- Cummings, P.T., see Lee, S.H. 293 (1998) 289
- Curioni, A., M. Boero and W. Andreoni,  $\text{Alq}_3$ : ab initio calculations of its structural and electronic properties in neutral and charged states 294 (1998) 263
- Curotto, E., D.L. Freeman, B. Chen and J.D. Doll, The melting transition of  $\text{Ni}_7$  and  $\text{Ni}_7\text{H}$  as modeled by a semi-empirical potential 295 (1998) 366
- Cyrier, M.C., see Haake, M. 292 (1998) 686
- Dabkara, N.K. and P.M. Agrawal, The maximum limit of rotational energy transfer in collisions of  $\text{N}_2$  with Ne and the power-gap law 299 (1999) 125
- Dachsel, H., see Müller, T. 293 (1998) 72
- Da Gama, A.A.S., see Parnaíba-daSilva, A.J. 296 (1998) 483
- Dagdigian, P.J., see Yang, X. 297 (1998) 506
- Dai, D., see Tan, H. 297 (1998) 173
- Dai, H., see Kong, J. 292 (1998) 567
- Dang, H., see Wang, X. 300 (1999) 739
- Danieli, R., see Tamassia, F. 300 (1999) 478
- Das, U.K. and P. Chaudhuri, Optical emission spectroscopic study of a radio-frequency plasma of  $\text{Ar} + \text{SiH}_4$  298 (1998) 211
- Da Silva, A.J.R., see Govind, N. 295 (1998) 129
- Datta, B., see Mahapatra, U.S. 299 (1999) 42
- Daudey, J.-P., see Ismail, N. 300 (1999) 296
- Dauw, X.L.R., see Bronsveld, M.V. 293 (1998) 528
- Davidson, E.R., see Jaręcki, A.A. 300 (1999) 44
- Davidson, E.R., see Staroverov, V.N. 296 (1998) 435
- Davies, P.B., see Fan, W.Y. 298 (1998) 222
- Davies, P.B., see Liu, Z. 291 (1998) 480
- Davis, W.W., see Moog, R.S. 299 (1999) 265
- Deàk, J.C., L.K. Iwaki and D.D. Dlott, When vibrations interact: ultrafast energy relaxation of vibrational pairs in polyatomic liquids 293 (1998) 405
- De Andrés, J., see Romero, T. 292 (1998) 323
- De Angelis, F., N. Re, A. Sgamellotti, A. Selloni, J. Weber and C. Floriani, A dynamical density functional study of CO migration in the Reppe carbonylation 291 (1998) 57
- Deb, B.M., see Roy, A.K. 292 (1998) 461
- Deb, B.M., see Singh, R. 296 (1998) 530
- De Beer, E., see Osborn, D.L. 292 (1998) 651
- De Belder, G., see Latterini, L. 295 (1998) 11
- Debnath, R., Observation of two different types of stable  $[\text{FeO}_4^-/\text{Na}^+]^0$  centres in a silica glass 291 (1998) 231



- DeClue, M.S., see Grunnet-Jepsen, A. 291 (1998) 553
- DeCristofano, B.S., see Venugopal Rao, S. 297 (1998) 491
- De Feyter, S., see Zhong, D. 298 (1998) 129
- Degli Esposti, C., see Bizzocchi, L. 293 (1998) 441
- De Groot, F.M.F., see Hu, Z. 297 (1998) 321
- De Groot, H.J.M., see La Penna, G. 294 (1998) 447
- De Kersabiec, A.-M., see Haouz, A. 294 (1998) 197
- De la Fuente, G.F., see Maser, W.K. 292 (1998) 587
- Delaire, J., see Dupuis, B. 300 (1999) 169
- De Lange, M.J.L., J.J. van Leuken, M.M.J.E. Drabbels, J. Bulhuis, J.G. Snijders and S. Stolte, Direct spectroscopic determination of the degree of orientation of parity-selected NO 294 (1998) 332
- De Langen, M. and K.O. Prins, Mobility of polyethylene chains in the orthorhombic and hexagonal phases investigated by NMR 299 (1999) 195
- De Leeuw, S.W., see Drukker, K. 291 (1998) 283
- De Leeuw, S.W., see Drukker, K. 298 (1998) 233
- Deleuze, M.S., see Pang, W.N. 296 (1998) 605
- Del Re, G., M. Brahimy and A. Peluso, A model for proton-assisted electron transfer 299 (1999) 511
- De Lucia, F.C., see Ball, C.D. 300 (1999) 227
- De Matteis, F., see Casalboni, M. 291 (1998) 167
- De Ménorval, L.-C., see Lamrabte, A. 295 (1998) 257
- De Mico, A., see Casalboni, M. 291 (1998) 167
- Demontis, P., see Fritzsche, S. 296 (1998) 253
- Demtröder, W., see Krämer, H.-G. 299 (1999) 212
- Demtröder, W., see Platz, T. 294 (1998) 397
- Den Hartog, F.T.H., M.P. Bakker, R.J. Silbey and S. Völker, Long-time spectral diffusion induced by short-time energy transfer in doped glasses: concentration-, wavelength- and temperature dependence of spectral holes 297 (1998) 314
- Denifl, G., see Brüning, F. 292 (1998) 177
- Dennis, K.W., see Chen, J.M. 294 (1998) 209
- Dentan, V., see Dupuis, B. 300 (1999) 169
- Depaemelaere, S., see Maus, M. 292 (1998) 115
- De Proft, F., see Boon, G. 295 (1998) 122
- De Proft, F., see Safi, B. 300 (1999) 85
- Dereñ, P.J., W. Stręk and J.-C. Krupa, Visible anti-Stokes emission of  $Gd^{3+}$  in  $Cs_2NaGdCl_6$  crystal 298 (1998) 217
- De Schryver, F.C., see Latterini, L. 295 (1998) 11
- De Schryver, F.C., see Maus, M. 292 (1998) 115
- De Schryver, F.C., see Rommens, J. 294 (1998) 434
- Desgroux, P., see Mercier, X. 299 (1999) 75
- Desmarais, N., C. Jamorski, F.A. Reuse and S.N. Khanna, Atomic arrangements in  $Ni_7$  and  $Ni_8$  clusters 294 (1998) 480
- De Sousa, A.R., see Sambrano, J.R. 294 (1998) 1
- Desvergne, J.P., see Zehnacker, A. 293 (1998) 357
- Dey, B.K., A. Askar and H. Rabitz, Alternating direction implicit technique and quantum evolution within the hydrodynamical formulation of Schrödinger's equation 297 (1998) 247
- Diau, E.W.-G., see Zhong, D. 298 (1998) 129
- Díaz-Megías, S. and L. Seijo, Wood-Boring ab initio model potential relativistic treatment of Ce and CeO 299 (1999) 613

- DiCésare, N., M. Belletête, M. Leclerc and G. Durocher, Thermochromic properties of quaterthiophene, an alkyl-substituted quaterthiophene derivative and its corresponding polymer 291 (1998) 487
- Dick, B., see Engert, J.M. 299 (1999) 423
- Dieckmann, T., see Wall, M.R. 291 (1998) 465
- Diehl, R.D., see Seyller, Th. 291 (1998) 567
- Dietrich, G., see Rousseau, R. 295 (1998) 41
- Díez López, M.-A., see García-Ochoa, I. 296 (1998) 335
- DiLabio, G.A. and J.S. Wright, Calculation of bond dissociation energies for large molecules using locally dense basis sets 297 (1998) 181
- Diller, R., Vibrational relaxation during the retinal isomerization in Bacteriorhodopsin 295 (1998) 47
- Ding, A., see Kanzow, H. 295 (1998) 525
- Dinis, C., see Becker, K.H. 300 (1999) 460
- Dixon, R.A., see Wee, A.T.S. 298 (1998) 146
- Glott, D.D., see Deák, J.C. 293 (1998) 405
- Doclo, K. and U. Röthlisberger, Ab initio molecular dynamics simulations of the gas-phase reaction of hydroxyl radical with nitrogen dioxide radical 297 (1998) 205
- Dolg, M., see Shukla, A. 294 (1998) 126
- Doll, J.D., see Curotto, E. 295 (1998) 366
- Domcke, W., see Sobolewski, A.L. 300 (1999) 533
- Domene, C., P.W. Fowler, P. Jemmer and P. Madden, Application of density functional theory to calculation of in-crystal anionic polarizability 299 (1999) 51
- Dong, R.Y., see Calucci, L. 296 (1998) 357
- Donker, H., see Kerp, H.R. 298 (1998) 302
- Donovan, R.J., see O'Keeffe, P. 298 (1998) 368
- Dopfer, O., R.V. Olkhov, D. Roth and J.P. Maier, Intermolecular interaction in proton-bound dimers. Infrared photodissociation spectra of  $Rg-HOCO^+$  ( $Rg = He, Ne, Ar$ ) complexes 296 (1998) 585
- Doran, S.J., see Wolber, J. 296 (1998) 391
- Dore, L., C.D. Esposti, A. Mazzavillani and G. Cazzoli, Pure rotational spectra of  $^{32}SD_3^+$  and  $^{34}SD_3^+$ . Determination of the substitution structure of the sulfonium ion 300 (1999) 489
- Douhal, A., see Chachisvilis, M. 293 (1998) 153
- Douhal, A., see García-Ochoa, I. 296 (1998) 335
- Dovesi, R., see Civalleri, B. 292 (1998) 394
- Drabbels, M.M.J.E., see de Lange, M.J.L. 294 (1998) 332
- Drachsel, W., see Adelt, M. 291 (1998) 425
- Dreier, T., see Schneider-Kühnle, Y. 294 (1998) 191
- Drewello, T., see Barrow, M.P. 293 (1998) 302
- Drichko, N.V., see Semkin, V.N. 295 (1998) 266
- Drukker, K. and S.W. de Leeuw, Corrigendum to "Molecular dynamics of an excess electron in aqueous solutions" [Chem. Phys. Lett. 291 (1998) 283] 298 (1998) 233
- Drukker, K. and S.W. de Leeuw, Molecular dynamics of an excess electron in aqueous solutions 291 (1998) 283
- Duan, C., see Zhang, W. 292 (1998) 133
- Dubernet, M.-L. and P.A. Tuckey, Raman  $Q$  and  $S$  line broadening and shifting coefficients: some commonly used assumptions revisited 300 (1999) 275
- Dulieu, O., see Gutterres, R.F. 300 (1999) 131
- Duncan, M.A., see Kirschner, K.N. 295 (1998) 204
- Dunsch, L., see Kuran, P. 292 (1998) 580

- Dupré, P., see Müller, T. 292 (1998) 243
- Dupuis, B., C. Michaut, I. Jouanin, J. Delaire, P. Robin, P. Feneyrou and V. Dentan, Photoinduced intramolecular charge-transfer systems based on porphyrin–viologen dyads for optical limiting 300 (1999) 169
- Dupuis, M., see Aida, M. 292 (1998) 474
- Dupuis, M., see Yamataka, H. 300 (1999) 583
- Durand, Ph., see Gemperle, F. 291 (1998) 517
- Düren, R., see Hauschildt, J. 300 (1999) 569
- Durocher, G., see DiCésare, N. 291 (1998) 487
- Durocher, G., see Shen, X. 298 (1998) 201
- Dusausoy, Y., see Tekely, P. 291 (1998) 471
- Düsterhöft, C., D. Heinemann and D. Kolb, Dirac–Fock–Slater calculations for diatomic molecules with a finite element defect correction method (FEM-DKM) 296 (1998) 77
- Dvoranová, D., see Brezová, V. 300 (1999) 667
- Dykstra, C.E., External electric field effects on the water trimer 299 (1999) 132
- Easter, D.C., Isomerization of isotopically-labeled benzene<sub>13</sub> during free jet expansion 297 (1998) 165
- Eckelt, J., see Yamaoka, H. 295 (1998) 245
- Eckert, H., see Chan, J.C.C. 292 (1998) 154
- Edelstein, J., see Keinan, S. 298 (1998) 43
- Edén, M. and M.H. Levitt, Excitation of carbon-13 triple quantum coherence in magic-angle-spinning NMR 293 (1998) 173
- Edholm, O., P.I. Ohlsson, M.L. Smith and J. Paul, The barrier for heme–protein separation estimated by non-equilibrium molecular dynamics simulations 291 (1998) 501
- Edman, L., S. Wennmalm, F. Tamsen and R. Rigler, Corrigendum to ‘‘Heterogeneity in single DNA conformational fluctuations’’. [Chem. Phys. Lett. 292 (1998) 15–21] 294 (1998) 625
- Edman, L., S. Wennmalm, F. Tamsen and R. Rigler, Heterogeneity in single DNA conformational fluctuations 292 (1998) 15
- Edwards, P.P., see Goldbach, A. 292 (1998) 137
- Egdell, R.G., see Wee, A.T.S. 298 (1998) 146
- Egorov, M.P., see Bagryansky, V.A. 295 (1998) 230
- Egorov, S.A. and J.L. Skinner, Semiclassical approximations to quantum time correlation functions 293 (1998) 469
- Ehara, M., see Lü, X. 291 (1998) 445
- Ehara, M., see Xu, X. 292 (1998) 282
- Ehrenfreund, E., see Lifshitz, E. 300 (1999) 626
- Eisenmenger, F., see Hansmann, U.H.E. 297 (1998) 374
- Eisenthal, K.B., see Srivastava, A. 292 (1998) 345
- Ellis, P.D., see Larsen, F.H. 292 (1998) 467
- Elmidaoui, A., see Lamrabte, A. 295 (1998) 257
- Emelianova, E.V., see Arkhipov, V.I. 296 (1998) 452
- Emsley, L., see Sakellariou, D. 293 (1998) 110
- Endo, H., see Yamaoka, H. 295 (1998) 245
- Engel, E., see Keller, S. 299 (1999) 165
- Engel, V., see Herwig, A. 300 (1999) 269
- Engel, V., see Rubner, O. 293 (1998) 485
- Engelhardt, G., see Markgraber, D. 300 (1999) 701
- Engert, J.M. and B. Dick, Measurement and assignment of the vibrationally resolved UV absorption spectrum of syn-methyl nitrite isolated in an argon matrix at 12 K 299 (1999) 423



- Engstrom, J.R., see Lam, A.M. 292 (1998) 229
- Enríquez, P.A., see González, M. 300 (1999) 603
- Epple, M., see Kuhnke, K. 294 (1998) 241
- Epstein, I.R., see Kurin-Csörgei, K. 295 (1998) 70
- Era, M., K. Maeda and T. Tsutsui, Enhanced phosphorescence from naphthalene-chromophore incorporated into lead bromide-based layered perovskite having organic-inorganic superlattice structure 296 (1998) 417
- Ernst, H., see Pingel, U.-T. 294 (1998) 345
- Ernst, R.R., see Fel'dman, E.B. 294 (1998) 297
- Erra Balsells, R., see Murgida, D.H. 294 (1998) 538
- Ertl, G., see Kelling, S. 293 (1998) 325
- Espinosa, E., C. Lecomte and E. Molins, Experimental electron density overlapping in hydrogen bonds: topology vs. energetics 300 (1999) 745
- Esposti, C.D., see Dore, L. 300 (1999) 489
- Eustatiu, I.G., T. Tyliczszak and A.P. Hitchcock, Inner-shell electron energy-loss spectroscopy of SF<sub>6</sub> at very high momentum transfer 300 (1999) 676
- Evans, C.M., R. Reininger and G.L. Findley, Photoionization spectra of CH<sub>3</sub>I perturbed by SF<sub>6</sub>: electron scattering in SF<sub>6</sub> gas 297 (1998) 127
- Evans, J.N.S., see Mitchell, D.J. 292 (1998) 656
- Fabeni, P., see Nikl, M. 291 (1998) 300
- Fabian, J.H., see Berger, R. 294 (1998) 363
- Falaras, P., see Provata, A. 297 (1998) 484
- Falcetta, M.F. and K.D. Jordan, Ab initio investigation of the temporary anion states of silane and the linear silanes: (Si<sub>n</sub>H<sub>2n+2</sub>), *n* = 2-5 300 (1999) 588
- Falcinelli, S., see Brunetti, B. 294 (1998) 584
- Falkovskaia, E., P.K. Sengupta and M. Kasha, Photophysical induction of dual fluorescence of quercetin and related hydroxyflavones upon intermolecular H-bonding to solvent matrix 297 (1998) 109
- Fally, S., see Bernath, P. 297 (1998) 293
- Fan, H.-J. and C.-W. Liu, Ab initio and DFT studies on the structure and binding interaction of M<sup>+</sup>CO<sub>2</sub> (M = Sc, Ti, ..., Zn) 300 (1999) 351
- Fan, L., Y. Li, F. Li, Y. Li and D. Zhu, Positive shifts of the C<sub>60</sub> reduction potentials by introducing cyano groups 294 (1998) 443
- Fan, W.Y., N.T. Hunt, Z. Liu and P.B. Davies, Infrared laser spectrum of high *J* pure rotational transitions of <sup>4</sup>HeD<sup>+</sup> 298 (1998) 222
- Fanourgakis, G.S., see Froudakis, G.E. 294 (1998) 109
- Farantos, S.C., see Froudakis, G.E. 294 (1998) 109
- Farmanara, P., see Radloff, W. 291 (1998) 173
- Fava, C., see Berardi, R. 297 (1998) 8
- Favero, P.G., see Caminati, W. 294 (1998) 377
- Fayer, M.D., see Aubuchon, C.M. 299 (1999) 84
- Fehrensens, B., D. Luckhaus and M. Quack, Mode selective stereomutation tunnelling in hydrogen peroxide isotopomers 300 (1999) 312
- Fehrensens, B., M. Hippler and M. Quack, Isotopomer-selective overtone spectroscopy by ionization detected IR + UV double resonance of jet-cooled aniline 298 (1998) 320
- Feigon, J., see Wall, M.R. 291 (1998) 465
- Fel'dman, E.B., R. Brüscheweiler and R.R. Ernst, From regular to erratic quantum dynamics in long spin 1/2 chains with an XY Hamiltonian 294 (1998) 297

- Feldman, V.I., F.F. Sukhov and A.Yu. Orlov, An ESR study of benzene radical cation in an argon matrix: evidence for favourable stabilization of  $^2B_{1g}$  rather than  $^2B_{2g}$  state 300 (1999) 713
- Fellows, C.E., see Gutterres, R.F. 300 (1999) 131
- Feneyrou, P., see Dupuis, B. 300 (1999) 169
- Feng, P.Y., M.Z. Liao and K. Balasubramanian, Low-lying electronic states of  $In_2As_2$ ,  $In_2As_2^+$  and  $In_2As_2^-$  296 (1998) 283
- Fernandez, C., see Pingel, U.-T. 294 (1998) 345
- Ferone, V., see Casalboni, M. 291 (1998) 167
- Ferramosche, R., see Brunetti, B. 294 (1998) 584
- Ferrari, A.C., see Barborini, E. 300 (1999) 633
- Ferrari, C., see Tombari, E. 300 (1999) 749
- Fick, D., see Jänsch, H.J. 296 (1998) 146
- Figari, G., see Magnasco, V. 291 (1998) 529
- Filatov, M. and W. Thiel, Tests of a density functional with Laplacian terms: activation barriers and bond-stretching energies 295 (1998) 467
- Filipponi, A., see Bowron, D.T. 293 (1998) 33
- Findley, G.L., see Evans, C.M. 297 (1998) 127
- Finlayson, B.A., see Scovell, D.L. 294 (1998) 255
- Finney, J.L., see Bowron, D.T. 293 (1998) 33
- Firth, S., see Walker, N.R. 292 (1998) 125
- Fischer, P., see Buckingham, A.D. 297 (1998) 239
- Fischer, R.A., see Schäfer, J. 300 (1999) 152
- Fisher, M.E. and D.M. Zuckerman, Chemical association via exact thermodynamic formulations 293 (1998) 461
- Fisher, M.L., see Colic, M. 291 (1998) 24
- Fishlock, T.W., see Wee, A.T.S. 298 (1998) 146
- Fisz, J.J., Flexible fluorophores as the probes for monitoring the structural and dynamical properties of organized molecular media 297 (1998) 409
- Fisz, J.J. and M. Buczkowski, Two-excited-state reversible reactions and fluorescence depolarization in uniaxially organized molecular media 296 (1998) 34
- Fitz Gerald, J., see Chen, Y. 299 (1999) 260
- Flahaut, E., A. Govindaraj, A. Peigney, Ch. Laurent, A. Rousset and C.N.R. Rao, Synthesis of single-walled carbon nanotubes using binary (Fe, Co, Ni) alloy nanoparticles prepared in situ by the reduction of oxide solid solutions 300 (1999) 236
- Flammang, R., P. Gerbaux and M.W. Wong, Identification of singlet and triplet SCNO<sup>+</sup> cations in the gas phase: theory and experiment 300 (1999) 183
- Flocke, N. and T.G. Schmalz, Valence bond multiple excitation RVB calculations on the singlet ground states of some carbon fullerenes  $C_n$  with  $20 \leq n \leq 60$  298 (1998) 71
- Floriani, C., see De Angelis, F. 291 (1998) 57
- Foley, H.C., see Stevens, M.G. 292 (1998) 352
- Fonseca, A., see Ahlskog, M. 300 (1999) 202
- Foord, J.S., see Wee, A.T.S. 298 (1998) 146
- Forberich, O., see Pfeiffer, T. 298 (1998) 351
- Forró, L., see Kamarás, K. 295 (1998) 279
- Fowler, C., see Shuali, Z. 300 (1999) 687
- Fowler, P.W., K.M. Rogers, G. Seifert, M. Terrones and H. Terrones, Pentagonal rings and nitrogen excess in fullerene-based BN cages and nanotube caps 299 (1999) 359
- Fowler, P.W., T. Heine, K.M. Rogers, J.P.B. Sandall, G. Seifert and F. Zerbetto,  $C_{36}$ , a hexavalent building block for fullerene compounds and solids 300 (1999) 369

- Fowler, P.W., see Domene, C. 299 (1999) 51
- Francisco, J.S., The structure and heat of formation of the  $\text{CH}_3\text{OCH}_2\text{O}$  radical 294 (1998) 319
- Francisco, J.S. and J.W. Thoman Jr., Adiabatic ionization potential and electron affinity of formaldehyde 300 (1999) 553
- Francisco, J.S., see Workman, M.A. 293 (1998) 65
- François, J.P., see Cai, Z.-L. 300 (1999) 69
- Frankland, S.J.V., see Mente, S. 293 (1998) 515
- Franks, K.J., see Li, H. 300 (1999) 247
- Frauenheim, T., see Jackson, K. 292 (1998) 235
- Freeman, D.L., see Curotto, E. 295 (1998) 366
- Freeman, R., see Linden, N. 296 (1998) 61
- Freude, D., see Pingel, U.-T. 294 (1998) 345
- Freund, H.-J., see Adelt, M. 291 (1998) 425
- Freund, H.-J., see Hill, T. 292 (1998) 524
- Freund, H.-J., see Klüner, T. 294 (1998) 413
- Freund, W.L., see Prater, K. 295 (1998) 82
- Frisch, M.J., see Wiberg, K.B. 297 (1998) 60
- Fritzsche, S., M. Wolfsberg, R. Haberlandt, P. Demontis, G.B. Suffritti and A. Tilocca, About the influence of lattice vibrations on the diffusion of methane in a cation-free LTA zeolite 296 (1998) 253
- Froudakis, G.E., G.S. Fanourgakis, S.C. Farantos and S.S. Xantheas, Binding energies and structures of  $\text{C}^+ \text{Ar}_n$  ( $n = 1-5$ ), clusters from first principles 294 (1998) 109
- Froudakis, G.E., see Andriotis, A.N. 292 (1998) 487
- Fthenakis, Z., see Andriotis, A.N. 292 (1998) 487
- Fujiki, M., see Toyoda, S. 293 (1998) 38
- Fujiki, S., see Kubozono, Y. 298 (1998) 335
- Fujisawa, J., Y. Ohba and S. Yamauchi, Pulsed and cw-time-resolved EPR studies of photoinduced electron transfer between zinc(II) porphyrin and fullerene 294 (1998) 248
- Fujishima, A., see Nakabayashi, S. 300 (1999) 409
- Fujita, N., see Sawamura, S. 299 (1999) 177
- Fujita, W., see Awaga, K. 293 (1998) 352
- Fujiwara, S., see Katoh, R. 291 (1998) 305
- Fujiyoshi, S., see Katoh, R. 292 (1998) 621
- Fukazawa, H., S. Mae, S. Ikeda and O. Watanabe, Proton ordering in Antarctic ice observed by Raman and neutron scattering 294 (1998) 554
- Fukui, K., I. Oshima, H. Oosterbeek and Y. Iwasawa, Reflection-absorption infrared spectroscopic study on a  $\text{CuO}_x/\text{SiO}_2$  model catalyst prepared by spin-coating on a  $\text{SiO}_2/\text{W}/\text{Si}(100)$  buried metal substrate 299 (1999) 158
- Fukumura, H., see Hatanaka, K. 300 (1999) 727
- Fukumura, H., see Saitow, K. 291 (1998) 433
- Fulde, P., H. Stoll and K. Kladko, On the ground state of solids with strong electron correlations 299 (1999) 481
- Fung, W.K.-M., see Wang, C.-R. 296 (1998) 505
- Furubayashi, M., see Yamaguchi, M. 298 (1998) 93
- Gadea, F.X., see Gemperle, F. 291 (1998) 517
- Gagliardi, L., see Skylaris, C.-K. 296 (1998) 445
- Gál, T., see March, N.H. 292 (1998) 384



- Gallagher Faeder, S.M., see Hybl, J.D. 297 (1998) 307
- Galyametdinov, Yu.G., see Binnemans, K. 300 (1999) 509
- Gannon, T.J., M. Tassotto and P.R. Watson, Orientation of molecules at a liquid surface revealed by ion scattering and recoiling spectroscopy 300 (1999) 163
- Gao, J.F., see Pang, W.N. 296 (1998) 605
- Gao, N.F., see Pang, W.N. 296 (1998) 605
- Gao, N.F., see Pang, W.N. 299 (1999) 207
- Gao, X.-C., H. Cao, C.-H. Huang, B.-G. Li, K. Ibrahim, F.-Q. Liu and S. Umitani, Electroluminescence from both a light-emitting layer and hole transport layer: spectral evidence for charge carrier tunneling injection 297 (1998) 530
- García-Moreno, I., see Arbeloa, T.L. 299 (1999) 315
- García-Muñoz, J.L., J. Cirujeda, J. Veciana and S.F.J. Cox, Magnetic transitions in the positional isomers (4-HOPNN and 2-HOPNN) of an organic nitronyl nitroxide radical using muon-spin rotation 293 (1998) 160
- García-Ochoa, I., M.-A. Díez López, M.H. Viñas, L. Santos, E. Martínez Ataz, F. Sánchez and A. Douhal, Hydrogen-bonding interactions and double proton-transfer reactions at both gates of cyclodextrins 296 (1998) 335
- García-Ochoa, I., see Chachisvilis, M. 293 (1998) 153
- Garg, A. and S.B. Sinnott, Effect of chemical functionalization on the mechanical properties of carbon nanotubes 295 (1998) 273
- Garland, N.L. and S.W. McElvany, Ionization potentials of TNAZ and its decomposition products 297 (1998) 147
- Garnache, A., A. Campargue, A.A. Kachanov and F. Stoeckel, Intracavity laser absorption spectroscopy near  $9400\text{ cm}^{-1}$  with a Nd:glass laser: application to  $^{14}\text{N}_2\text{ }^{16}\text{O}$  292 (1998) 698
- Garrone, E., see Civalleri, B. 294 (1998) 103
- Garrone, E., see Civalleri, B. 299 (1999) 443
- Garscadden, A., see Jiao, C.Q. 297 (1998) 121
- Gast, P., see Proskuryakov, I.I. 299 (1999) 566
- Gauss, J., O. Christiansen and J.F. Stanton, Triple excitation effects in coupled-cluster calculations of frequency-dependent hyperpolarizabilities 296 (1998) 117
- Gauss, J., see Christiansen, O. 292 (1998) 437
- Gdanitz, R.J., Corrigendum to "Accurately solving the electronic Schrödinger equation of atoms and molecules using explicitly correlated ( $r_{12}$ -)MR-CI: the ground state potential energy curve of  $\text{N}_2$ " [Chem. Phys. Lett. 283 (1998) 253] 295 (1998) 540
- Ge, J.-Y. and J.Z.H. Zhang, Channel-dependent complex absorbing potential for multi-channel scattering 292 (1998) 51
- Ge, Q., see Brown, W.A. 299 (1999) 253
- Gee, C., P. Boissel and G. Ohanessian, Metal-acetylene binding in gaseous  $\text{WC}_2\text{H}_2^+$  298 (1998) 85
- Geerlings, P., see Boon, G. 295 (1998) 122
- Geerlings, P., see Safi, B. 300 (1999) 85
- Geiger, H., see Becker, K.H. 300 (1999) 460
- Gemperle, F., F.X. Gadea and Ph. Durand, Non-optimized complex absorbing potentials for quantum resonances 291 (1998) 517
- Geng, J., T. Kobayashi and M. Takami, Evaluation of absolute optical oscillator strengths for transitions from the A-state to the  $np$  Rydberg series in NO 291 (1998) 277
- Georges, R., see Bach, M. 294 (1998) 533
- Geppi, M., see Calucci, L. 296 (1998) 357
- Gerbaux, P., see Flammang, R. 300 (1999) 183

- Gerber, Ch., see Berger, R. 294 (1998) 363
- Gerber, G., see Simon, M. 296 (1998) 579
- Gerber, R.B., see Broude, S. 299 (1999) 437
- Gerdts, T. and U. Manthe, A microscopic description of dissipation in systems with strong vibronic coupling: the  $S_1$  and  $S_2$  absorption spectra of pyrazine 295 (1998) 167
- Gerhards, M., M. Schiwiek, C. Unterberg and K. Kleinermanns, OH stretching vibrations in aromatic cations: IR/PIRI spectroscopy 297 (1998) 515
- Gerhards, M., S. Schumm, C. Unterberg and K. Kleinermanns, Structure and vibrations of catechol in the  $S_1$  state and ionic ground state 294 (1998) 65
- Ghiggino, K.P., see Scholes, G.D. 292 (1998) 601
- Ghosh, S., see Bhattacharyya, S. 297 (1998) 154
- Giaquinta, P.V., see Costa, D. 291 (1998) 252
- Giaquinta, P.V., see Costa, D. 299 (1999) 252
- Gilat, S.L., see Owrutsky, J.C. 293 (1998) 555
- Gillbro, T., see Ma, Y.-Z. 300 (1999) 465
- Giménez, X., see Huarte-Larrañaga, F. 291 (1998) 346
- Gimzewski, J.K., see Berger, R. 294 (1998) 363
- Girolami, G.S., see Awaga, K. 293 (1998) 352
- Gobetto, R., see Asaro, F. 300 (1999) 414
- Goldbach, A., P.D. Barker, P.A. Anderson and P.P. Edwards, The clusters  $Cd_2^{2+}$  and  $Cd_4^{2+}$  in zeolite A 292 (1998) 137
- Goldfield, E.M., see Meijer, A.J.H.M. 293 (1998) 270
- Gomes, P.A.J., see Varandas, A.J.C. 297 (1998) 458
- Gong, Q., see Zhang, T. 298 (1998) 236
- González, M., D. Troya, M.P. Puyuelo, R. Sayós and P.A. Enríquez, The dynamics of the  $O(^1D) + N_2O \rightarrow NO + NO$  reaction revisited: a QCT study on model potential energy surfaces 300 (1999) 603
- Goodman, L., see Wiedmann, R.T. 293 (1998) 391
- Goodson, B.M., see Haake, M. 292 (1998) 686
- Gopinath, C.S., R. Muthukumaran, L.L. Welling, M.A. Bennett and P.T. Manoharan, X-ray photoelectron spectroscopic studies on binuclear gold(II) complexes 296 (1998) 566
- Gorceac, L.L., see Klokishner, S.I. 300 (1999) 613
- Gotō, H., A frontier mode-following method for mapping saddle points of conformational interconversion in flexible molecules starting from the energy minimum 292 (1998) 254
- Gough, T.E., T.E. Rowat and R. Illner, Modeling the solid state reaction  $CO_2 \cdot C_2H_2 \rightarrow CO_2 + C_2H_2$  298 (1998) 196
- Govind, N., Y.A. Wang, A.J.R. da Silva and E.A. Carter, Accurate ab initio energetics of extended systems via explicit correlation embedded in a density functional environment 295 (1998) 129
- Govindaraj, A., see Flahaut, E. 300 (1999) 236
- Govindaraj, A., see Satishkumar, B.C. 293 (1998) 47
- Govindaraj, A., see Satishkumar, B.C. 300 (1999) 473
- Grabowska, A., see Borowicz, P. 291 (1998) 351
- Grabowski, I., see Meissner, L. 300 (1999) 53
- Graja, A., see Semkin, V.N. 295 (1998) 266
- Gray, S.K., see Meijer, A.J.H.M. 293 (1998) 270
- Grebenschikov, S.Yu., see Hauschildt, J. 300 (1999) 569
- Greve, T., see Natterer, J. 293 (1998) 455
- Grigorenko, B.L., A.V. Nemukhin and N.V. Ozhegova, MD-DIM simulations of the  $^3\Pi_g(\text{ion-pair}) \rightarrow ^3\Pi_u(\text{valence})$  red-shifted transitions of  $Cl_2$  in neon matrices 296 (1998) 84

- Grimme, S., Continuous symmetry measures for electronic wavefunctions 297 (1998) 15
- Gritsenko, O.V., N.A. Cordero, A. Rubio and J.A. Alonso, Gradient correction to the exchange pair-correlation function of the weighted spin-density approximation in the density functional formalism 296 (1998) 307
- Groenen, E.J.J., see Bronsveld, M.V. 293 (1998) 528
- Grotjahn, D.B., see Allen, M.D. 293 (1998) 397
- Grün, M., see Tanaka, H. 293 (1998) 541
- Grunnet-Jepsen, A., D. Wright, B. Smith, M.S. Bratcher, M.S. DeClue, J.S. Siegel and W.E. Moerner, Spectroscopic determination of trap density in C<sub>60</sub>-sensitized photorefractive polymers 291 (1998) 553
- Gu, G., see He, L. 300 (1999) 504
- Gu, Y., see Wang, B. 300 (1999) 99
- Gu, Z., see Wang, X. 300 (1999) 739
- Guan, W., T. Matsumoto and T. Kawai, Time- and space-resolved diagnosis of laser ablation plasma probed by optical transmittance 291 (1998) 161
- Guerrero, H.M., R.L. Cappelletti, D.A. Neumann and T. Yildirim, Structure and lattice dynamics of K<sub>1</sub>C<sub>60</sub> in the orthorhombic phase: a neutron scattering study 297 (1998) 265
- Guihéry, N., see Miguel, B. 294 (1998) 49
- Guldi, D.M., see Brezová, V. 300 (1999) 667
- Güntherodt, H.-J., see Berger, R. 294 (1998) 363
- Guo, L.-P., see Ren, H.-L. 292 (1998) 317
- Gütlich, P., see Ksenofontov, V. 294 (1998) 545
- Gutman, I., T. Soldatović and D. Vidović, The energy of a graph and its size dependence. A Monte Carlo approach 297 (1998) 428
- Gutowski, M. and P. Skurski, Electron binding energies in linear dipole-bound (HCN)<sub>n</sub><sup>-</sup> (n = 2-5) anions 300 (1999) 331
- Gutsev, G.L., P. Jena and R.J. Bartlett, Electric quadrupole moments and electron affinities of atoms from H to Cl: a coupled-cluster study 291 (1998) 547
- Gutsev, G.L., P. Jena and R.J. Bartlett, Structure and stability of BF<sub>3</sub>\*F and AlF<sub>3</sub>\*F superhalogens 292 (1998) 289
- Gutterres, R.F., M. Argollo de Menezes, C.E. Fellows and O. Dulieu, Generalized simulated annealing method in the analysis of atom-atom interaction 300 (1999) 131
- Ha, T.-K. and J. Makarewicz, Ab initio potential energy surface and rovibrational states of HBO 299 (1999) 637
- Ha, T.-K., see Nguyen, M.T. 293 (1998) 90
- Haake, M., B.M. Goodson, D.D. Laws, E. Brunner, M.C. Cyrier, R.H. Havlin and A. Pines, NMR of supercritical laser-polarized xenon 292 (1998) 686
- Haaland, P.D., see Jiao, C.Q. 297 (1998) 121
- Haberlandt, R., see Fritzsche, S. 296 (1998) 253
- Hachiya, N., see Umemoto, H. 296 (1998) 203
- Haddon, R.C., see Chen, Y. 299 (1999) 532
- Hafner, J.H., M.J. Bronikowski, B.R. Azamian, P. Nikolaev, A.G. Rinzler, D.T. Colbert, K.A. Smith and R.E. Smalley, Catalytic growth of single-wall carbon nanotubes from metal particles 296 (1998) 195
- Hager, G.D., see Herbelin, J.M. 299 (1999) 583
- Hahn, S. and G. Stock, Efficient calculation of time- and frequency-resolved spectra: a mixed non-perturbative/perturbative approach 296 (1998) 137



- Halac, E., E. Burgos and H. Bonadeo, Molecular structure and dynamical properties of  $C_{36}$ : a semi-empirical calculation 299 (1999) 64
- Halac, E., see Burgos, E. 298 (1998) 273
- Halas, N.J., see Westcott, S.L. 300 (1999) 651
- Halkier, A., S. Coriani and P. Jørgensen, The molecular electric quadrupole moment of  $N_2$  294 (1998) 292
- Halkier, A., see Coriani, S. 293 (1998) 324
- Halpern, J.B., see Rudert, A.D. 294 (1998) 381
- Hamilton, I.P., Comment on "Are the Bader Laplacian and the Bohm quantum potential equivalent?" 297 (1998) 261
- Hamilton, I.P., see Chan, W.-T. 292 (1998) 57
- Hamilton, I.P., see Chan, W.-T. 297 (1998) 217
- Hammerum, S., Heats of formation and proton affinities by the G3 method 300 (1999) 529
- Hammes-Schiffer, S., see Soudackov, A.V. 299 (1999) 503
- Hamon, M.A., see Chen, Y. 299 (1999) 532
- Han, K.-L., see Zhang, H. 300 (1999) 483
- Han, W., Y. Bando, K. Kurashima and T. Sato, Boron-doped carbon nanotubes prepared through a substitution reaction 299 (1999) 368
- Han, Y.-K., see Lee, H.-S. 293 (1998) 97
- Hancock, G., see Bakker, B.L.G. 294 (1998) 565
- Handy, N.C., see Skylaris, C.-K. 296 (1998) 445
- Hansmann, U.H.E., F. Eisenmenger and Y. Okamoto, Stochastic dynamics simulations in a new generalized ensemble 297 (1998) 374
- Haouz, A., C. Twist, C. Zentz, A.-M. de Kersabiec, S. Pin and B. Alpert, Förster energy transfer from tryptophan to flavin in glucose oxidase enzyme 294 (1998) 197
- Harigaya, K., Optical excitations in fractal antenna supermolecules with conjugated electrons: extended dendrimers 300 (1999) 33
- Harikumar, K.R., see Satishkumar, B.C. 300 (1999) 473
- Härle, H., A. Lehnert, U. Metka, H.-R. Volpp, L. Willms and J. Wolfrum, In-situ detection of chemisorbed CO on a polycrystalline platinum foil using infrared-visible sum-frequency generation 293 (1998) 26
- Harper, J., see Presilla-Márquez, J.D. 300 (1999) 719
- Harris, P.J.F. and S.C. Tsang, A simple technique for the synthesis of filled carbon nanoparticles 293 (1998) 53
- Harrison, R.J., see Müller, T. 293 (1998) 72
- Hasegawa, J., see Nakatsuji, H. 296 (1998) 499
- Hasegawa, K., T. Ono, Y. Inoue and M. Kusunoki, Spin-exchange interactions in the  $S_2$ -state manganese tetramer in photosynthetic oxygen-evolving complex deduced from  $g = 2$  multiline EPR signal 300 (1999) 9
- Häser, M., see Weigend, F. 294 (1998) 143
- Hashimoto, N., K. Someda and K. Yamanouchi, Probing intramolecular vibrational energy re-distribution by using a pair of femtosecond-laser pulses: a theoretical model 291 (1998) 130
- Hashimoto, T., see Choe, Y.-K. 295 (1998) 380
- Hatanaka, K., T. Itoh, T. Asahi, N. Ichinose, S. Kawanishi, T. Sasuga, H. Fukumura and H. Masuhara, Time-resolved ultraviolet-visible absorption spectroscopic study on femtosecond KrF laser ablation of liquid benzyl chloride 300 (1999) 727
- Hättig, C., Dispersion formulas for the second hyperpolarizability components  $\gamma_{||}$ ,  $\gamma_{\perp}$  and  $\gamma_K$  296 (1998) 245
- Hättig, C., see Coriani, S. 293 (1998) 324

- Hättig, C., see Larsen, H. 291 (1998) 536
- Hauge, R.H., see Mickelson, E.T. 296 (1998) 188
- Häupl, T., T. Zimmermann, R. Hermann and O. Brede, The photoisomerization of spiro[cyclohexadiene-indoline] via an intramolecular charge transfer state 291 (1998) 215
- Hauschildt, J., J. Weiß, C. Beck, S.Yu. Grebenshchikov, R. Düren, R. Schinke and J. Koput, Unimolecular dissociation of HOCl: unexpectedly broad distribution of rate constants 300 (1999) 569
- Hauser, A., see Schenker, S. 297 (1998) 281
- Havlas, Z., see Hobza, P. 299 (1999) 180
- Havlin, R.H., see Haake, M. 292 (1998) 686
- Havlin, S., see Canpolat, M. 294 (1998) 9
- Hayakawa, F., see Lee, G.H. 299 (1999) 309
- Hayakawa, F., see Negishi, Y. 294 (1998) 370
- Hayashi, S., Differential broadening between the signals split by the residual dipolar interaction with  $^{14}\text{N}$  in  $^{13}\text{C}$  CP/MAS NMR spectra of nitroanilines 299 (1999) 272
- Hayes, J.M., see Reinot, T. 299 (1999) 410
- Hayes, R.A., see Howard, S.T. 293 (1998) 523
- He, G.-Z., see Zhang, H. 300 (1999) 483
- He, J., C. Ma and A.S.-C. Cheung, Wavelength-resolved laser-induced fluorescence study of the  $\text{A}^2\Pi-\text{X}^2\Sigma$  transition of  $\text{ZrN}$ : vibrational constants of  $\text{A}^2\Pi$  and  $\text{X}^2\Sigma$  states 295 (1998) 535
- He, L., Z.X. Shen, G. Gu, L. Qin and S.H. Tang, Luminescence due to the indirect band-gap transition activated by the inter-valence transition of Se clusters confined in 13X zeolite 300 (1999) 504
- He, R.R., H.Z. Jin, J. Zhu, Y.J. Yan and X.H. Chen, Physical and electronic structure in carbon nanotubes 298 (1998) 170
- He, T., see Li, L. 291 (1998) 179
- Heath, J.R., see Remacle, F. 291 (1998) 453
- Heemeier, M., see Hill, T. 292 (1998) 524
- Heidelberg, C., J. Schroeder, D. Schwarzer and V.S. Vikhrenko, Mode specificity of vibrational energy relaxation of azulene in  $\text{CO}_2$  at low and high density 291 (1998) 333
- Hein, J., see Paa, W. 292 (1998) 607
- Heine, T., see Fowler, P.W. 300 (1999) 369
- Heinemann, D., see Düsterhöft, C. 296 (1998) 77
- Helbig, M., see Paa, W. 292 (1998) 607
- Held, A., L.Ya. Baranov, H.L. Selzle and E.W. Schlag, Lifetime control in Rydberg states using fast switching DC electric fields II. Enhancement for nitric oxide 291 (1998) 318
- Held, A., U. Aigner, L.Ya. Baranov, H.L. Selzle and E.W. Schlag, Lifetime control in Rydberg states. An application to the autoionizing series below the  $^2\text{P}_{1/2}$  ionization limit of xenon 299 (1999) 110
- Held, A., see Baranov, L.Ya. 291 (1998) 311
- Helgaker, T., see Ruud, K. 297 (1998) 467
- Hellgren, N., see Suenaga, K. 300 (1999) 695
- Henshaw, T.L., see Herbelin, J.M. 299 (1999) 583
- Henton, S., M. Islam and I.W.M. Smith, Intramolecular V-V transfer between the components of the  $(3_1/2_14_15_1)$  and  $(3_14_1/2_14_25_1)$  Fermi dyads in acetylene in  $\text{C}_2\text{H}_2-\text{C}_2\text{H}_2$  collisions 291 (1998) 223
- Hepp, M., F. Herregodts and M. Herman, Fourier transform infrared jet spectroscopy using a heated slit source 294 (1998) 528

- Hepp, M., see Bach, M. 294 (1998) 533  
 Hepp, M., see Roth, D.A. 298 (1998) 381  
 Herbelin, J.M., T.L. Henshaw, B.D. Rafferty, B.T. Anderson, R.F. Tate, T.J. Madden, G.C. Manke II and G.D. Hager, The measurement of gain on the 1.315  $\mu\text{m}$  transition of atomic iodine in a subsonic flow of chemically generated  $\text{NCl}(a^1\Delta)$  299 (1999) 583  
 Herman, M., see Bach, M. 294 (1998) 533  
 Herman, M., see Hepp, M. 294 (1998) 528  
 Herman, P., see Konopasek, I. 293 (1998) 429  
 Hermann, R., see Häupl, T. 291 (1998) 215  
 Hermans, C., see Bernath, P. 297 (1998) 293  
 Hermans, L.J.F., see Il'ichov, L.V. 297 (1998) 439  
 Hermans, L.J.F., see Nagels, B. 294 (1998) 387  
 Hernadi, K., see Ahlskog, M. 300 (1999) 202  
 Hernández, E., see Ramírez, R. 291 (1998) 44  
 Herrebout, W.A., A.A. Stolov, E.J. Sluyts and B.J. van der Veken, FTIR spectra of liquid argon/liquid nitrogen mixtures: evidence for the existence of a 1:1 bonded species  $\text{Ar} \cdot \text{N}_2$  295 (1998) 223  
 Herregodts, F., see Hepp, M. 294 (1998) 528  
 Hershberger, J.F., see Park, J. 295 (1998) 89  
 Herwig, A., M. Braun and V. Engel, Structures in molecular photofragment and photoelectron distributions from two-photon non-resonant excitation 300 (1999) 269  
 Hess, B.A., see Malkina, O.L. 296 (1998) 93  
 Hess, P., see Wetterauer, U. 300 (1999) 397  
 Heully, J.-L., see Ismail, N. 300 (1999) 296  
 Hewett, K.B. and D.W. Setser, Generation of  $\text{NBr}(a^1\Delta)$  by the reaction of  $\text{N}_3$  radicals with Br atoms: a flow reactor source for quenching rate constant measurements 297 (1998) 335  
 Heydtmann, H., see Nölle, A. 299 (1999) 561  
 Hihara, T., S. Pokrant and J.A. Becker, Magnetic moments and chemical bonding in isolated  $\text{Bi}_N\text{Co}_M$  clusters 294 (1998) 357  
 Hikida, T., T. Ibuki and K. Okada,  $\text{C}_6\text{F}_5\text{X}$  ( $\text{X} = \text{H}, \text{F}, \text{Cl}, \text{Br}$  and  $\text{I}$ ) excited radical cation formation in the 10–40 eV region 292 (1998) 638  
 Hilczer, M. and M. Tachiya, Effect of solvent polarity on the potential of mean force between two molecular ions: MD simulation 295 (1998) 337  
 Hill, T., M. Mozaffari-Afshar, J. Schmidt, T. Risse, S. Stempel, M. Heemeier and H.-J. Freund, Influence of CO adsorption on the magnetism of small Co particles deposited on  $\text{Al}_2\text{O}_3$  292 (1998) 524  
 Hillier, I.H., see Wright, K. 299 (1999) 527  
 Hino, S., K. Umishita, K. Iwasaki, T. Miyamae, M. Inakuma and H. Shinohara, Ultraviolet photoelectron spectra of  $\text{Sc}@C_{82}$  300 (1999) 145  
 Hippler, M., see Fehrensén, B. 298 (1998) 320  
 Hirao, K., see Choe, Y.-K. 295 (1998) 380  
 Hirao, K., see Nakayama, K. 300 (1999) 303  
 Hiraoka, K., T. Sugiyama, J. Katsuragawa and S. Yamabe, How are CO molecules bound to  $\text{NO}^+$ ? Shell formation of the gas-phase cluster ions of  $\text{NO}^+(\text{CO})_n$  with  $n = 4$  and 8 299 (1999) 545  
 Hiraoka, K., see Kubozono, Y. 298 (1998) 335  
 Hirata, F., see Chong, S.-H. 293 (1998) 119  
 Hirata, F., see Kinoshita, M. 297 (1998) 433



- Hirata, Y., T. Okada and T. Nomoto, Photophysical properties of diphenylacetylene derivatives in the solution phase: Comparison with the dynamical properties of diphenylbutadiyne 293 (1998) 371
- Hiratsuka, H., see Okutsu, T. 299 (1999) 597
- Hirayama, S., see Niikura, H. 296 (1998) 343
- Hishikawa, A., see Sako, T. 294 (1998) 571
- Hishiki, T., see Yanagi, H. 292 (1998) 332
- Hitchcock, A.P., see Eustatiu, I.G. 300 (1999) 676
- Hitchcock, A.P., see Neville, J.J. 300 (1999) 451
- Ho, K.M., see Pan, B.C. 292 (1998) 75
- Hobza, P., V. Špirko, Z. Havlas, K. Buchhold, B. Reimann, H.-D. Barth and B. Brutschy, Anti-hydrogen bond between chloroform and fluorobenzene 299 (1999) 180
- Hodgkinson, P., see Sakellariou, D. 293 (1998) 110
- Hof, T., see Jänsch, H.J. 296 (1998) 146
- Hoff, A.J., see Proskuryakov, I.I. 299 (1999) 566
- Hoffmann, M.R., see Khait, Y.G. 300 (1999) 289
- Hogervorst, W., see Reinhold, E. 296 (1998) 411
- Hogiu, S., see Pfeiffer, M. 295 (1998) 56
- Holleman, I., see von Helden, G. 299 (1999) 171
- Holloway, J.H., see Cooke, S.A. 298 (1998) 151
- Holloway, J.H., see Waclawik, E.R. 295 (1998) 289
- Holmes, S.M., see Awaga, K. 293 (1998) 352
- Holmes, W., see Aubuchon, C.M. 299 (1999) 84
- Holmgren, L., M. Andersson and A. Rosén, NO on copper clusters 296 (1998) 167
- Holmlid, L., see Wang, J. 295 (1998) 500
- Honda, Y. and H. Nakatsuji, Force concept for predicting the geometries of molecules in an external electric field 293 (1998) 230
- Hong, M., see Sandström, D. 300 (1999) 213
- Honma, K., see Kawamoto, Y. 298 (1998) 227
- Hoppmeier, M., see Zimmer, K. 293 (1998) 366
- Hore, P.J., see Till, U. 298 (1998) 7
- Hou, H., see Wang, B. 300 (1999) 99
- Houjou, H., K. Koyama, M. Wada, K. Sameshima, Y. Inoue and M. Sakurai, Effects of the protein electrostatic environment on the absorption maximum of bacteriorhodopsin 294 (1998) 162
- Howard, S.T., R.A. Hayes and M.B. Hursthouse, Polarizabilities of alkylsiloxanate and methoxysiloxanate anions 293 (1998) 523
- Hoz, S., see Basch, H. 294 (1998) 117
- Hsiao, C.-C., see Kumar, A. 297 (1998) 300
- Hu, A., P. Otto and J. Ladik, Relativistic all-electron Hartree–Fock–Dirac calculation of a quasi one-dimensional chain of selenium atoms 293 (1998) 277
- Hu, C., see Wei, X. 300 (1999) 385
- Hu, H., see Chen, Y. 299 (1999) 532
- Hu, W., see Zhou, S. 297 (1998) 77
- Hu, Z., C. Mazumdar, G. Kaindl, F.M.F. de Groot, S.A. Warda and D. Reinen, Valence electron distribution in  $\text{La}_2\text{Li}_{1/2}\text{Cu}_{1/2}\text{O}_4$ ,  $\text{Nd}_2\text{Li}_{1/2}\text{Ni}_{1/2}\text{O}_4$ , and  $\text{La}_2\text{Li}_{1/2}\text{Co}_{1/2}\text{O}_4$  297 (1998) 321
- Hu, Z., see Meier, R. 292 (1998) 507
- Hua, D. and J. Luo, An investigation of the potentiostatic current oscillation during the anodic dissolution of iron in sulfuric acid 299 (1999) 345

- Huang, C.-H., see Gao, X.-C. 297 (1998) 530  
Huang, M.-B., see Wang, Z.-X. 291 (1998) 381  
Huarte-Larrañaga, F., X. Giménez, A. Aguilar and M. Baer, On the accuracy of reactive scattering calculations with absorbing potentials: a new implementation based on a generalized R-matrix propagation 291 (1998) 346  
Huber, J.R., see Radloff, W. 291 (1998) 173  
Hübner, O., V. Termath, A. Berning and J. Sauer, A CASSCF/ACPF study of spectroscopic properties of FeS and FeS<sup>-</sup> and the photoelectron spectrum of FeS<sup>-</sup> 294 (1998) 37  
Huffman, C.B., see Mickelson, E.T. 296 (1998) 188  
Huh, S.H., see Lee, G.H. 299 (1999) 309  
Hultman, L., see Suenaga, K. 300 (1999) 695  
Hunt, N.T., see Fan, W.Y. 298 (1998) 222  
Hursthouse, M.B., see Howard, S.T. 293 (1998) 523  
Hybl, J.D., A.W. Albrecht, S.M. Gallagher Faeder and D.M. Jonas, Two-dimensional electronic spectroscopy 297 (1998) 307  
Hynes, A.J., R.C. Richter, A.R. Rosendahl and C.D. Clark, S<sub>2</sub> (a <sup>1</sup>Δ) production in the photolysis of reduced sulfides: production chemistry, spectroscopy and interference potential in the LIF detection of OH 295 (1998) 25  
  
Iachello, F., see Müller, T. 292 (1998) 243  
Iachello, F., see Sako, T. 299 (1999) 35  
Ibrahim, K., see Gao, X.-C. 297 (1998) 530  
Ibrahim, M., see Müller, T. 292 (1998) 243  
Ibuki, T., see Hikida, T. 292 (1998) 638  
Ichihashi, T., see Yudasaka, M. 299 (1999) 91  
Ichikawa, T., see Takada, T. 300 (1999) 253  
Ichimura, T., see Omori, T. 293 (1998) 436  
Ichinose, N., see Hatanaka, K. 300 (1999) 727  
Ichinose, N., see Saitow, K. 291 (1998) 433  
Ide, T., see Miyasaka, H. 292 (1998) 339  
Iijima, S., see Yudasaka, M. 299 (1999) 91  
Iijima, T., Convergence in the calculation of X-ray scattering intensities from liquids 299 (1999) 488  
Iiyama, T., see Tanaka, H. 293 (1998) 541  
Ikai, M., see Moriwaki, K. 292 (1998) 500  
Ikeda, S., see Fukazawa, H. 294 (1998) 554  
Ikeda, T., see Kodaira, T. 300 (1999) 499  
Ikemoto, I., see Ishihara, S. 295 (1998) 475  
Il'ichov, L.V., L.J.F. Hermans, A.M. Shalagin and P.L. Chapovsky, Direct optical enrichment of nuclear spin isomers of molecules 297 (1998) 439  
Illas, F., see Lopez, N. 294 (1998) 611  
Illas, F., see Mele, F. 295 (1998) 409  
Illenberger, E., see Brüning, F. 292 (1998) 177  
Illenberger, E., see Le Coat, Y. 296 (1998) 208  
Illner, R., see Gough, T.E. 298 (1998) 196  
Imamura, A., see Yamazaki, T. 295 (1998) 431  
Imamura, Y., S. Ten-no, K. Yonemitsu and Y. Tanimura, Theoretical study on electron correlation of 1-D (DCNQI)<sub>2</sub>M (M = Li, Ag) salts 298 (1998) 15  
Inakuma, M., see Hino, S. 300 (1999) 145

- Inakuma, M., see Nishibori, E. 298 (1998) 79
- Inakuma, M., see Wang, C.-R. 300 (1999) 379
- Ingólfsson, O., see Le Coat, Y. 296 (1998) 208
- Inokuma, K., see Nakabayashi, S. 294 (1998) 204
- Inomata, S., see Yamaguchi, M. 298 (1998) 93
- Inoue, Y., see Hasegawa, K. 300 (1999) 9
- Inoue, Y., see Houjou, H. 294 (1998) 162
- Inoue, Y., see Saito, N. 297 (1998) 72
- Inoue, Y., see Yamane, T. 291 (1998) 137
- Ioannou, A.G., see Skylaris, C.-K. 296 (1998) 445
- Ishchenko, V.N., S.A. Kochubei, V.I. Makarov and I.V. Khmelinskii, On cooling of vibrationally excited benzene molecules in supersonic molecular beams 299 (1999) 227
- Ishida, T. and G.C. Schatz, Monte Carlo sampling methods for determining potential energy surfaces using Shepard interpolation. The  $\text{O}(\text{}^1\text{D}) + \text{H}_2$  system 298 (1998) 285
- Ishihara, S., I. Ikemoto, S. Suzuki, K. Kikuchi, Y. Achiba and T. Kobayashi, Relaxation dynamics of photoexcitations in  $\text{C}_{60}$  films 295 (1998) 475
- Ishikawa, M., see Ohtani, H. 299 (1999) 571
- Ishikawa, Y., see Vilkas, M.J. 296 (1998) 68
- Ishitobi, H., Z. Sekkat and S. Kawata, Individualized optically induced orientation of photochemical isomers 300 (1999) 421
- Islam, M., see Henton, S. 291 (1998) 223
- Ismail, N., J.-L. Heully, T. Saue, J.-P. Daudey and C.J. Marsden, Theoretical studies of the actinides: method calibration for the  $\text{UO}_2^{2+}$  and  $\text{PuO}_2^{2+}$  ions 300 (1999) 296
- Itaya, A., see Miyasaka, H. 292 (1998) 339
- Itkis, M.E., see Chen, Y. 299 (1999) 532
- Itoh, K., see Ohkata, Y. 295 (1998) 17
- Itoh, M., see Ohta, N. 292 (1998) 535
- Itoh, T., see Hatanaka, K. 300 (1999) 727
- Iucci, G., see Polzonetti, G. 292 (1998) 515
- Iwai, K., see Maus, M. 292 (1998) 115
- Iwaki, L.K., see Deàk, J.C. 293 (1998) 405
- Iwasa, Y., see Kubozono, Y. 298 (1998) 335
- Iwasaki, K., see Hino, S. 300 (1999) 145
- Iwasawa, Y., see Fukui, K. 299 (1999) 158
- Iwata, S., see Vener, M.V. 292 (1998) 87
- Jabalameli, A., R. Venkatraman, A. Nowek and R.H. Sullivan, Molecular complexes of nitric acid with  $\text{N}_2$ : a post Hartree-Fock quantum mechanical study 295 (1998) 135
- Jabs, W., see Koput, J. 295 (1998) 462
- Jackson, B., see Shalashilin, D.V. 291 (1998) 143
- Jackson, K., G. Jungnickel and T. Frauenheim, Cage-forming tendencies in  $\text{Si}_n\text{N}_m$  clusters 292 (1998) 235
- Jacoby, G., see Roeselová, M. 293 (1998) 309
- Jacques, P., see Burget, D. 291 (1998) 207
- Jagličić, Z., see Mrzel, A. 298 (1998) 329
- Jakobsen, H.J., see Larsen, F.H. 292 (1998) 467
- Jakobsen, M., see Ruoff, P. 291 (1998) 249
- Jamali, J.B., N. Wada, Y. Shimobe, N. Achiwa, S. Kuwajima, Y. Soejima and K. Mukai, The effect of non-magnetic impurities on the spin-Peierls transition of 3-(4-cyanophenyl)-1,5-dimethyl-6-oxoverdazyl radical crystal, p-CyDOV 292 (1998) 661



- Jamnik, A., Sedimentation equilibrium of adhesive spheres in a planar gap 292 (1998) 481
- Jamorski, C., see Desmarais, N. 294 (1998) 480
- Jander, P., see Küick, S. 300 (1999) 189
- Janot, J.-M., see Lamrabte, A. 295 (1998) 257
- Jänsch, H.J., T. Hof, U. Ruth, J. Schmidt, D. Stahl and D. Fick, NMR of surfaces: sub-monolayer sensitivity with hyperpolarized  $^{129}\text{Xe}$  296 (1998) 146
- Jantoljak, H., see Kuhlmann, U. 294 (1998) 237
- Jaręcki, A.A. and E.R. Davidson, Density functional theory calculations for  $\text{F}^-$  300 (1999) 44
- Jarid, A., see Anane, H. 296 (1998) 277
- Jarolímek, O., see Nikl, M. 291 (1998) 300
- Jarvis, G.K. and R.P. Tuckett, On the adiabatic ionisation energy of the  $\text{CF}_3$  free radical 295 (1998) 145
- Jasny, J., see Vdovin, A. 296 (1998) 557
- Jastrzębski, W., see Pashov, A. 292 (1998) 615
- Jeannin, C., see Portella-Oberli, M.T. 296 (1998) 323
- Jeloica, L. and V. Sidis, DFT investigation of the adsorption of atomic hydrogen on a cluster-model graphite surface 300 (1999) 157
- Jemmer, P., see Domene, C. 299 (1999) 51
- Jena, P., see Gutsev, G.L. 291 (1998) 547
- Jena, P., see Gutsev, G.L. 292 (1998) 289
- Jena, P., see Weber, S.E. 295 (1998) 175
- Jenouvrier, A., see Bernath, P. 297 (1998) 293
- Jerschow, A., Multiple echoes initiated by a single radio frequency pulse in NMR 296 (1998) 466
- Jeschke, G. and H.W. Spiess, NMR-correlated high-field electron paramagnetic resonance spectroscopy 293 (1998) 9
- Jeschke, G. and R. Bittl, Electron spin echo envelope modulation by electronic spin-spin interactions in radical pairs undergoing electron transfer 294 (1998) 323
- Jett, S.D., see Balzer, F. 297 (1998) 273
- Ji, X., see Moore, P.B. 296 (1998) 259
- Jian, H., see Zhang, T. 298 (1998) 236
- Jiao, C.Q., A. Garscadden and P.D. Haaland, Ion chemistry in octafluorocyclobutane,  $c\text{-C}_4\text{F}_8$  297 (1998) 121
- Jigato, M.P., D.A. King and A. Yoshimori, The chemisorption of spin polarised NO on  $\text{Ag}\{111\}$  300 (1999) 639
- Jin, H.Z., see He, R.R. 298 (1998) 170
- Jirsak, T., see Rodriguez, J.A. 296 (1998) 421
- Jochims, H.W., see Boyle, K.J. 294 (1998) 507
- Johann, C., S.H. Patil, K.T. Tang and J.P. Toennies, Asymptotic theory for the  $^2\Sigma$  Van der Waals potentials of alkali dimer cations 295 (1998) 158
- Johansson, M.P., see Suenaga, K. 300 (1999) 695
- Johnson, M.A., see Kim, J. 297 (1998) 90
- Jokisaari, J., see Vaara, J. 296 (1998) 541
- Jonas, D.M., see Hybl, J.D. 297 (1998) 307
- Jones, W., see Kaneyoshi, M. 296 (1998) 183
- Joos, S., see Achatz, U. 291 (1998) 459
- Jordan, K.D., see Falcetta, M.F. 300 (1999) 588
- Jordan, K.D., see Pedulla, J.M. 291 (1998) 78
- Jørgensen, P., see Coriani, S. 293 (1998) 324
- Jørgensen, P., see Coriani, S. 300 (1999) 61

- Jørgensen, P., see Halkier, A. 294 (1998) 292
- Jørgensen, P., see Larsen, H. 291 (1998) 536
- Jortner, J., see Metzler, R. 293 (1998) 477
- Jouanin, I., see Dupuis, B. 300 (1999) 169
- Journet, C., see Kuhlmann, U. 294 (1998) 237
- Jung, J.O., see Broude, S. 299 (1999) 437
- Jungnickel, G., see Jackson, K. 292 (1998) 235
- Jungwirth, P., see Roeselová, M. 293 (1998) 309
- Jungwirth, P., see Slavíček, P. 300 (1999) 561
- Jürgensen, A., see Neville, J.J. 300 (1999) 451
- Jursic, B.S., Complete basis set ab initio computational study of unimolecular decomposition of dimethyl ether 295 (1998) 447
- Jursic, B.S., Density functional theory exploring the HONO potential energy surface 299 (1999) 334
- Kable, S.H., see Schmidt, T.W. 292 (1998) 80
- Kachanov, A.A., see Garnache, A. 292 (1998) 698
- Kaczmarek, Ł., see Borowicz, P. 291 (1998) 351
- Kageyama, T., see Okutsu, T. 299 (1999) 597
- Kago, K., see Yamaoka, H. 295 (1998) 245
- Kahn, O., see Ksenofontov, V. 294 (1998) 545
- Kain, J.S., see Császár, A.G. 293 (1998) 317
- Kaindl, G., see Hu, Z. 297 (1998) 321
- Kaindl, G., see Meier, R. 292 (1998) 507
- Kajimoto, O., see Kometani, N. 294 (1998) 619
- Kakitani, T., see Kimura, A. 298 (1998) 241
- Kakudate, Y., see Katoh, R. 291 (1998) 305
- Kaldor, U., see Roeselová, M. 293 (1998) 309
- Kamarás, K., S. Pekker, L. Forró and D.B. Tanner, Infrared and optical spectra of polymerized AC<sub>60</sub> fullerenes 295 (1998) 279
- Kamiya, N., see Ohtani, H. 299 (1999) 571
- Kanada, T., see Ohta, N. 292 (1998) 535
- Kanaev, A.V., see Monticone, S. 295 (1998) 237
- Kaneko, K., see Tanaka, H. 293 (1998) 541
- Kaneko, M., see Ohtani, H. 299 (1999) 571
- Kaneyoshi, M. and W. Jones, Exchange of interlayer terephthalate anions from a Mg–Al layered double hydroxide: formation of intermediate interstratified phases 296 (1998) 183
- Kang, H., H.W. Lee, W.R. Cho and S.M. Lee, Molecular shape effect in polyatomic ion–surface scattering. Surface-induced dissociation of Fe(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub><sup>+</sup> and FeC<sub>5</sub>H<sub>5</sub><sup>+</sup> at Si(100) 292 (1998) 213
- Kanno, H., K. Tomikawa and O. Mishima, Raman spectra of low- and high-density amorphous ices 293 (1998) 412
- Kan'no, K., see Akimoto, I. 292 (1998) 561
- Kanzow, H., A. Schmalz and A. Ding, Laser-assisted production of multi-walled carbon nanotubes from acetylene 295 (1998) 525
- Kaplan, A., see Lifshitz, E. 300 (1999) 626
- Kar, T., see Sannigrahi, A.B. 299 (1999) 518
- Karimi-Nejad, Y., F. Löhr, D. Schipper, H. Rüterjans and R. Boelens, Gradient-purged isotope filter experiments for the detection of bound water in proteins 300 (1999) 706

- Karpfen, A., The intermolecular interaction between amines and  $F_2$ . An ab initio study 299 (1999) 493
- Karyakina, E.L., see Andrievsky, G.V. 300 (1999) 392
- Kasha, M., see Falkovskaia, E. 297 (1998) 109
- Kashihara, S., see Nagamura, T. 294 (1998) 167
- Kashino, S., see Kubozono, Y. 298 (1998) 335
- Kashino, S., see Yoshida, Y. 291 (1998) 31
- Kasuya, A., see Saito, Y. 294 (1998) 593
- Kasuya, A., see Sugano, M. 292 (1998) 575
- Katada, M., see Sueki, K. 300 (1999) 140
- Kato, H. and A. Kudo, New tantalate photocatalysts for water decomposition into  $H_2$  and  $O_2$  295 (1998) 487
- Kato, M., Y. Nanba and Y. Taniguchi, Erratum to: "Effect of water and deuterated water on Raman spectra of chloroacetone: evidence for the conformational effect on hydration". [Chem. Phys. Lett. 289 (1998) 30-34] 294 (1998) 626
- Kato, S., see Nakamura, H. 297 (1998) 187
- Kato, R. and M. Kotani, Fluorescence from the second excited state of an anthracene crystal observed by two-step excitation 300 (1999) 734
- Kato, R., H. Yokoi, S. Usuba, Y. Kakudate and S. Fujiwara, Excitation density effect on the decomposition of liquid benzene by ArF excimer laser (193 nm) irradiation 291 (1998) 305
- Kato, R., S. Fujiyoshi and M. Kotani, Observation of weak fluorescence from the second excited state in an anthracene crystal 292 (1998) 621
- Katsuragawa, J., see Hiraoka, K. 299 (1999) 545
- Katz, G., see Zeiri, Y. 300 (1999) 523
- Kauffman, J.F., see Khajepour, M. 297 (1998) 141
- Kauffman, J.M., see Vdovin, A. 296 (1998) 557
- Kaukasoina, P., see Seyller, Th. 291 (1998) 567
- Kaupp, M., see Malkina, O.L. 296 (1998) 93
- Kawai, H., see Nagamura, T. 294 (1998) 167
- Kawai, T., see Guan, W. 291 (1998) 161
- Kawakami, Y., see Seko, T. 291 (1998) 438
- Kawamata, H., see Negishi, Y. 294 (1998) 370
- Kawamoto, Y. and K. Honma, Fluorescence excitation spectrum of Ni-Ar complex 298 (1998) 227
- Kawanishi, S., see Hatanaka, K. 300 (1999) 727
- Kawanishi, S., see Saitow, K. 291 (1998) 433
- Kawasaki, M., see Umemoto, H. 296 (1998) 203
- Kawashima, J., see Nakatsuji, S. 296 (1998) 159
- Kawata, S., see Ishitobi, H. 300 (1999) 421
- Kaya, K., see Lee, G.H. 299 (1999) 309
- Kaya, K., see Negishi, Y. 294 (1998) 370
- Kedziora, G.S., see Müller, T. 293 (1998) 72
- Keil, M., see Krämer, H.-G. 299 (1999) 212
- Keinan, S., M. Pinsky, M. Plato, J. Edelstein and D. Avnir, Quantitative evaluation of the near- $C_2$  symmetry of the bacterial photosynthetic reaction center 298 (1998) 43
- Keir, R.I., see Lamb, D.W. 291 (1998) 197
- Keller, S. and E. Engel, Quantum theory of fast electron impact ionization of  $C_{60}$ : application of the spherical jellium model 299 (1999) 165
- Kelling, S., S. Cerasari, H.H. Rotermund, G. Ertl and D.A. King, A photoemission electron microscopy (PEEM) study of the effect of surface acoustic waves on catalytic CO oxidation over Pt{110} 293 (1998) 325



- Kellö, V. and A.J. Sadlej, The quadrupole moment of the  $^{39}\text{K}$  and  $^{41}\text{K}$  nuclei from microwave data for KF and KCl 292 (1998) 403
- Kemper, P.R., P. Weis and M.T. Bowers,  $\text{Ni}^+(\text{H}_2)_n$ : Ligand bond energies for ground state ions 293 (1998) 503
- Kennedy, G.R., C.-L. Ning and J. Pfab, The 355 nm photodissociation of jet-cooled  $\text{CH}_3\text{SNO}$ : alignment of the NO photofragment 292 (1998) 161
- Kentgens, A.P.M. and R. Verhagen, Advantages of double frequency sweeps in static, MAS and MQMAS NMR of spin  $I = 3/2$  nuclei 300 (1999) 435
- Kern, K., see Kuhnke, K. 294 (1998) 241
- Kerp, H.R., H. Donker, R.B.M. Koehorst, T.J. Schaafsma and E.E. van Faassen, Exciton transport in organic dye layers for photovoltaic applications 298 (1998) 302
- Keshavamurthy, S., Scaling of the average survival probability for low dimensional systems 300 (1999) 281
- Khairallah, G. and J.B. Peel, Identification of dianions of  $\text{C}_{84}$  and  $\text{C}_{90}$  by electrospray mass spectrometry 296 (1998) 545
- Khait, Y.G. and M.R. Hoffmann, Analytic derivative methods for evaluating nonadiabatic coupling matrix elements within the SC-QDPT method 300 (1999) 289
- Khajepour, M. and J.F. Kauffman, Chain relaxation kinetics in the intramolecular charge transfer reaction of 1-(9-anthryl)-3-(4-dimethylaniline)propane in supercritical  $\text{CO}_2$ : bulk solvent properties characterize reactivity 297 (1998) 141
- Khan, M.I., G.C. Bazan and Z.D. Popovic, Evidence for electric field-assisted dissociation of the excited singlet state into charge carriers in MEH-PPV 298 (1998) 309
- Khanna, S.N., see Desmarais, N. 294 (1998) 480
- Khetrapal, C.L., N. Suryaprakash and S. Vivekanandan, Nematic mixture methods for the determination of chemical shift anisotropy 296 (1998) 537
- Khmelniskii, I.V., see Ishchenko, V.N. 299 (1999) 227
- Kiefer, W., see Loo, B.H. 297 (1998) 83
- Kiefer, W., see Urlaub, E. 298 (1998) 177
- Kiguchi, M., see Terada, S. 300 (1999) 645
- Kikuchi, K., see Ishihara, S. 295 (1998) 475
- Kikuchi, K., see Sueki, K. 291 (1998) 37
- Kikuchi, K., see Sueki, K. 300 (1999) 140
- Kilic, H.S., see Singhal, R.P. 292 (1998) 643
- Kim, E.H., see Osborn, D.L. 292 (1998) 651
- Kim, H., S. Shin and K.J. Shin, A test of the boundary doubling method for the numerical solution of diffusion-reaction systems 291 (1998) 341
- Kim, J., I. Becker, O. Cheshnovsky and M.A. Johnson, Photoelectron spectroscopy of the 'missing' hydrated electron clusters  $(\text{H}_2\text{O})_n^-$ ,  $n = 3, 5, 8$  and  $9$ : Isomers and continuity with the dominant clusters  $n = 6, 7$  and  $\geq 11$  297 (1998) 90
- Kim, K., see Pedulla, J.M. 291 (1998) 78
- Kim, K.-H., B. Lee and S. Lee, Structures and spectroscopic properties of  $\text{SC}_n\text{S}$  ( $n = 2-6$ ): density functional theory study 297 (1998) 65
- Kim, M.C., see Lee, H.-S. 293 (1998) 97
- Kim, O.-K., see Clays, K. 293 (1998) 337
- Kim, O.-K., see Owrutsky, J.C. 293 (1998) 555
- Kim, S.K., see Yoon, M.-C. 300 (1999) 207
- Kimura, A. and T. Kakitani, Nonperturbative method of electron transfer via a midway molecule 298 (1998) 241

- King, D.A., see Brown, W.A. 299 (1999) 253
- King, D.A., see Jigato, M.P. 300 (1999) 639
- King, D.A., see Kelling, S. 293 (1998) 325
- King, D.A., see Sharma, R.K. 291 (1998) 1
- King, K.D., see Alexander, U.N. 299 (1999) 291
- Kinoshita, M., Y. Okamoto and F. Hirata, Singular behavior of the reference interaction site model theory observed for peptide in salt solution 297 (1998) 433
- Kinugawa, K., Path integral centroid molecular dynamics study of the dynamic structure factors of liquid para-hydrogen 292 (1998) 454
- Kira, A., see Wang, Y. 299 (1999) 576
- Kirkwood, J.C., D.J. Ulness and A.C. Albrecht, On the mechanism of vibrational dephasing in liquid benzene by coherent anti-Stokes Raman scattering using incoherent light 293 (1998) 167
- Kirkwood, J.C., D.J. Ulness, A.C. Albrecht and M.J. Stimson, Raman spectrograms in fifth order coherent Raman scattering: The sequential CARS process in liquid benzene 293 (1998) 417
- Kirschner, K.N., B. Ma, J.P. Bowen and M.A. Duncan, Theoretical investigation of the  $\text{Ca}^+-\text{N}_2$  and  $\text{Ca}^{2+}-\text{N}_2$  complexes 295 (1998) 204
- Kisiel, Z. and L. Pszczółkowski, Rotational spectrum and spectroscopic constants of  $^{36}\text{Ar} \cdots \text{H}^{35}\text{Cl}$  and  $^{40}\text{Ar} \cdots \text{HCl}$  291 (1998) 190
- Kitagawa, H., see Kubozono, Y. 298 (1998) 335
- Kitajima, Y., see Adachi, J. 294 (1998) 559
- Kitajima, Y., see Terada, S. 300 (1999) 645
- Kladko, K., see Fulde, P. 299 (1999) 481
- Klafter, J., see Metzler, R. 293 (1998) 477
- Klein, S., M.J. Bearpark, B.R. Smith, M.A. Robb, M. Olivucci and F. Bernardi, Mixed state 'on the fly' non-adiabatic dynamics: the role of the conical intersection topology 292 (1998) 259
- Kleinerhmanns, K., see Gerhards, M. 294 (1998) 65
- Kleinerhmanns, K., see Gerhards, M. 297 (1998) 515
- Klenina, I.B., see Proskuryakov, I.I. 299 (1999) 566
- Klinowski, J., see Zhou, W. 292 (1998) 207
- Klochkov, V.K., see Andrievsky, G.V. 300 (1999) 392
- Kloepfer, J.A., V.H. Vilchiz, V.A. Lenchenkov and S.E. Bradforth, Femtosecond dynamics of photodetachment of the iodide anion in solution: resonant excitation into the charge-transfer-to-solvent state 298 (1998) 120
- Klokishner, S.I. and L.L. Gorceac, Nuclear quadrupole resonance of mixed-valence charge-ordered dimers 300 (1999) 613
- Klüner, T., S. Thiel, H.-J. Freund and V. Staemmler, The vibrational excitation of NO desorbing from NiO(100) after UV laser irradiation: is  $\text{NO}^-$  a possible intermediate species? 294 (1998) 413
- Knochenmuss, R., Excited-state proton transfer in 1-naphthol  $\cdot (\text{NH}_3)_n$  complexes: the threshold size is  $n = 4$  293 (1998) 191
- Knowles, P.J., see Manby, F.R. 296 (1998) 1
- Knyukshto, V., E. Zenkevich, E. Sagun, A. Shulga and S. Bachilo, Unusual dynamic relaxation of triplet-excited *meso*-phenyl-substituted porphyrins and their chemical dimers at room temperatures 297 (1998) 97
- Kobayashi, T., see Geng, J. 291 (1998) 277
- Kobayashi, T., see Ishihara, S. 295 (1998) 475
- Kobayashi, T., see Sugita, A. 296 (1998) 365
- Koc, K., see Vilkas, M.J. 296 (1998) 68

- Koch, H., see Pedersen, T.B. 293 (1998) 251
- Kochubei, S.A., see Ishchenko, V.N. 299 (1999) 227
- Koda, S., see Koga, K. 293 (1998) 180
- Kodaira, T., T. Ikeda and H. Takeo, Incorporation of AgI clusters into the cages of zeolites LTA and FAU observed by optical spectra and X-ray diffraction patterns 300 (1999) 499
- Koehorst, R.B.M., see Kerp, H.R. 298 (1998) 302
- Koga, K., A. Takami and S. Koda, IR spectra of H<sub>2</sub>S isolated in free-standing crystals of Kr and Xe 293 (1998) 180
- Koga, T., see Matsuyama, H. 300 (1999) 515
- Kogej, T., D. Beljonne, F. Meyers, J.W. Perry, S.R. Marder and J.L. Brédas, Mechanisms for enhancement of two-photon absorption in donor-acceptor conjugated chromophores 298 (1998) 1
- Köhler, J., see van Oijen, A.M. 292 (1998) 183
- Koizumi, H., see Takada, T. 300 (1999) 253
- Kolb, D., see Düsterhöft, C. 296 (1998) 77
- Kolb, D., see v. Kopylow, A. 295 (1998) 439
- Kolessov, A., see Liu, K. 299 (1999) 374
- Kolos, R., Photolysis of dicyanodiacetylene in argon matrices 299 (1999) 247
- Koma, A., see Shimada, T. 291 (1998) 419
- Komaguchi, K., T. Kumada, T. Takayanagi, Y. Aratono, M. Shiotani and T. Miyazaki, H atom-H<sub>2</sub> molecule van der Waals complexes in solid argon matrix by high-resolution ESR spectroscopy 300 (1999) 257
- Komatsu, K., see Ohtsuki, T. 300 (1999) 661
- Komatsu, T., see Yudasaka, M. 299 (1999) 91
- Kometani, N., H. Nakajima, K. Asami, Y. Yonezawa and O. Kajimoto, Excited-state dynamics of the mixed J-aggregate of two kinds of cyanine dyes in layer-by-layer alternate assemblies 294 (1998) 619
- Komorowski, L., see Ordon, P. 292 (1998) 22
- Konarev, D.V., see Semkin, V.N. 295 (1998) 266
- Kong, J., A.M. Cassell and H. Dai, Chemical vapor deposition of methane for single-walled carbon nanotubes 292 (1998) 567
- Kong, W., see Li, H. 300 (1999) 247
- Konings, R.J.M., A.S. Booij and A. Kovács, The infrared spectra of SeO<sub>2</sub> and TeO<sub>2</sub> in the gas phase 292 (1998) 447
- Konopasek, I., P. Kvasnicka, P. Herman, H. Linnertz, T. Obsil, J. Vecer, J. Svobodova, K. Strzalka, L. Mazzanti and E. Amler, The origin of the diphenylhexatriene short lifetime component in membranes and solvents 293 (1998) 429
- Koput, J., W. Jabs and M. Winnewisser, An ab initio study on the equilibrium structure and torsional potential energy function of carbodiimide 295 (1998) 462
- Koput, J., see Hauschildt, J. 300 (1999) 569
- Kornweitz, H. and R.D. Levine, Formation of molecular iodine in high-energy four-center CH<sub>3</sub>I + CH<sub>3</sub>I collisions 294 (1998) 153
- Kosloff, R., see Zeiri, Y. 300 (1999) 523
- Kosmidis, C., see Singhal, R.P. 292 (1998) 643
- Köster, A.M., see Martínez, A. 299 (1999) 630
- Kosugi, K., T. Nakabayashi and N. Nishi, Low-frequency Raman spectra of crystalline and liquid acetic acid and its mixtures with water. Is the liquid dominated by hydrogen-bonded cyclic dimers? 291 (1998) 253
- Kosugi, N., see Adachi, J. 294 (1998) 559



- Kotani, M., see Katoh, R. 292 (1998) 621  
 Kotani, M., see Katoh, R. 300 (1999) 734  
 Kotani, M., see Ono, M. 295 (1998) 493  
 Kotani, M., see Ono, M. 295 (1998) 34  
 Kounose, N., see Okutsu, T. 299 (1999) 597  
 Kovačević, B., Z.B. Maksić and P. Rademacher, High basicity of alkylated 2-tetrazenes: an ab initio study 293 (1998) 245  
 Kovács, A., see Konings, R.J.M. 292 (1998) 447  
 Kowalczyk, P., see Pashov, A. 292 (1998) 615  
 Koyama, K., see Houjou, H. 294 (1998) 162  
 Koyama, K., see Saito, N. 300 (1999) 262  
 Koyama, Y., see Sashima, T. 299 (1999) 187  
 Kozlov, A.A., see Tameev, A.R. 294 (1998) 605  
 Kraka, E., see Cremer, D. 292 (1998) 97  
 Krämer, H.-G., M. Keil, C.B. Suarez, W. Demtröder and W. Meyer, Vibrational structures in the  $A^2E'' \leftarrow X^2E'$  system of the lithium trimer: high-resolution spectroscopy and ab initio calculations 299 (1999) 212  
 Kramer, M.J., see Chen, J.M. 294 (1998) 209  
 Krastev, I., see Nakabayashi, S. 294 (1998) 204  
 Kraus, D., R.J. Saykally and V.E. Bondybey, Cavity ringdown laser absorption spectra of tungsten oxide 295 (1998) 285  
 Krause, M., see Kuran, P. 292 (1998) 580  
 Krause, P.J., D.C. Clary, D.T. Anderson, M.W. Todd, R.L. Schwartz and M.I. Lester, Time-resolved dissociation of the  $H_2$ -OH entrance channel complex 294 (1998) 518  
 Krawczyk, S., Excited states and electrochromism of radical cation of the carotenoid astaxanthin 294 (1998) 351  
 Kremer, K., see Mooney, D.A. 294 (1998) 135  
 Krishna, M.M.G. and N. Periasamy, Orientational distribution of linear dye molecules in bilayer membranes 298 (1998) 359  
 Krishnan, V., see Sen, A. 294 (1998) 499  
 Krissinel, E.B., see Agmon, N. 294 (1998) 79  
 Kristyan, S. and M.C. Lin, Theoretical calculations for the kinetics of the  $HN + NO$  reaction 297 (1998) 200  
 Kroes, G.-J., see McCormack, D.A. 296 (1998) 515  
 Krokidis, X., B. Silvi and M.E. Alikhani, Topological characterization of the isomerization mechanisms in  $XNO$  ( $X = H, Cl$ ) 292 (1998) 35  
 Krückeberg, S., see Rousseau, R. 295 (1998) 41  
 Krüger, S., see Pacchioni, G. 299 (1999) 137  
 Krumscheid, C., see Nölle, A. 299 (1999) 561  
 Krupa, J.-C., see Dereñ, P.J. 298 (1998) 217  
 Krupa, J.-C., see Zhang, W. 292 (1998) 133  
 Ksenofontov, V., G. Levchenko, H. Spiering, P. Gütllich, J.-F. Létard, Y. Bouhedja and O. Kahn, Spin crossover behavior under pressure of  $Fe(PM-L)_2(NCS)_2$  compounds with substituted 2'-pyridylmethylene 4-anilino ligands 294 (1998) 545  
 Kubach, C., see Rougeau, N. 299 (1999) 120  
 Kubo, S., see Yoshioka, Y. 294 (1998) 459  
 Kubozono, Y., S. Fujiki, K. Hiraoka, T. Urakawa, Y. Takabayashi, S. Kashino, Y. Iwasa, H. Kitagawa and Y. Mitani, Raman study of  $Cs_3C_{60}$  under ambient pressure 298 (1998) 335

- Kubozono, Y., see Yoshida, Y. 291 (1998) 31
- Kück, S. and P. Jander, Luminescence from  $V^{3+}$  in tetrahedral oxo-coordination 300 (1999) 189
- Kudo, A., see Kato, H. 295 (1998) 487
- Kudoh, S., M. Takayanagi and M. Nakata, Conformational cooling in a supersonic jet of 1,2-dichloroethane studied by matrix isolation infrared spectroscopy 296 (1998) 329
- Kuhlmann, U., H. Jantoljak, N. Pfänder, P. Bernier, C. Journet and C. Thomsen, Infrared active phonons in single-walled carbon nanotubes 294 (1998) 237
- Kuhn, P.S., Y. Levin and M.C. Barbosa, Complex formation between polyelectrolytes and ionic surfactants 298 (1998) 51
- Kuhnke, K., M. Epple and K. Kern, Second-harmonic spectroscopy of fullerenes 294 (1998) 241
- Kuki, M., see Sashima, T. 299 (1999) 187
- Kumada, T., see Komaguchi, K. 300 (1999) 257
- Kumar, A., C.-C. Hsiao, Y.-Y. Lee and Y.-P. Lee, Observation of saturation dip in degenerate four-wave mixing and two-color resonant four-wave mixing spectra of jet-cooled CH 297 (1998) 300
- Kumar, G.R. and D. Mathur, Reply to Comment on "On the ionization and dissociation of  $NO_2$  by short, intense laser pulses" 292 (1998) 647
- Kummrow, A., see Pfeiffer, M. 295 (1998) 56
- Kumzerov, Yu.A., see Semkin, V.N. 295 (1998) 266
- Kuppermann, A., see Billing, G.D. 294 (1998) 26
- Kuran, P., M. Krause, A. Bartl and L. Dunsch, Preparation, isolation and characterisation of  $Eu@C_{74}$ : the first isolated europium endohedral fullerene 292 (1998) 580
- Kurashima, K., see Han, W. 299 (1999) 368
- Kurin-Csörgei, K., M. Orbán, A.M. Zhabotinsky and I.R. Epstein, On the nature of patterns arising during polymerization of acrylamide in the presence of the methylene blue-sulfide-oxygen oscillating reaction 295 (1998) 70
- Kurosaki, Y. and T. Takayanagi, A direct isomerization path for the  $H_6^+$  cluster. An ab initio molecular orbital study 293 (1998) 59
- Kurosaki, Y. and T. Takayanagi, A theoretical study on an isotope effect in the  $CH_3 + H_2 \rightarrow CH_4 + H$  reaction 299 (1999) 57
- Kusunoki, M., see Hasegawa, K. 300 (1999) 9
- Kuwahara, D., T. Nakai and S. Miyajima, Two-dimensional NMR measurements of heteronuclear dipolar powder spectra using the chemical-shift-anisotropy recovery technique 291 (1998) 244
- Kuwajima, S., see Jamali, J.B. 292 (1998) 661
- Kuzik, L.A., see Alieva, E.V. 292 (1998) 542
- Kvasnicka, P., see Konopasek, I. 293 (1998) 429
- Ladik, J., see Hu, A. 293 (1998) 277
- Lægsgaard, E., see Pedersen, M.Ø. 299 (1999) 403
- Laenen, R. and K. Simeonidis, Energy relaxation and reorientation of the OH mode of simple alcohol molecules in different solvents monitored by transient IR spectroscopy 299 (1999) 589
- Laenen, R. and K. Simeonidis, Vibrational energy migration in a hydrogen-bonded dimer probed with ultrafast time-resolved spectroscopy 292 (1998) 631
- Lahmani, F., see Zehnacker, A. 293 (1998) 357
- Laitenberger, P., see Thomas, P.J. 294 (1998) 229
- Lallemand, J.-Y., see Abergel, D. 298 (1998) 257
- Lam, A.M., Y.-J. Zheng and J.R. Engstrom, The effect of strain on gas-surface reactivity in group-IV heteroepitaxial systems 292 (1998) 229

- Lam, S.K. and D. Lo, Delayed luminescence spectroscopy and optical phase conjugation in eosin Y-doped sol-gel silica glasses 297 (1998) 329
- Lamb, D.W., R.I. Keir and G.L.D. Ritchie, Polarizability and magnetizability anisotropies of trimethylboroxine,  $\text{Me}_3\text{B}_3\text{O}_3$ . Comparison of boroxine and benzene ring systems 291 (1998) 197
- Lampre, I., D. Markovitsi, A. Sharonov and M. Veber, Triarylpyrylium salts: dynamics of the monomer-dimer equilibrium via a triplet absorption study 293 (1998) 423
- Lamrabte, A., J.-M. Janot, A. Elmidaoui, P. Seta, L.-C. de Ménorval, R. Backov, J. Rozière, J.-L. Sauvajol and J. Allègre, Evidence of confinement of fullerene  $\text{C}_{60}$  in microporous VPI-5 zeolite 295 (1998) 257
- Lang, B., see Simon, M. 296 (1998) 579
- Lang, H.P., see Berger, R. 294 (1998) 363
- Langenaeker, W., see Boon, G. 295 (1998) 122
- Langley, A.J., see Singhal, R.P. 292 (1998) 643
- Lankers, M., see Urlaub, E. 298 (1998) 177
- La Penna, G., F. Buda, A. Bifone and H.J.M. de Groot, The transition state in the isomerization of rhodopsin 294 (1998) 447
- Lapinski, L. and M. Vala, Linear  $\text{C}_{11}$  cluster: an isotopic infrared study 300 (1999) 195
- Larsen, F.H., H.J. Jakobsen, P.D. Ellis and N.Chr. Nielsen, Molecular dynamics from  $^2\text{H}$  Quadrupolar Carr-Purcell-Meiboom-Gill solid-state NMR spectroscopy 292 (1998) 467
- Larsen, H., C. Hättig, J. Olsen and P. Jørgensen, A basis set study of coupled cluster and full configuration interaction calculations of molecular electric properties for BH 291 (1998) 536
- Larsen, R.E. and R.M. Stratt, Mutual-nearest-neighbor pairs in fluids 297 (1998) 211
- Larson, C.W., see Presilla-Márquez, J.D. 300 (1999) 719
- Latterini, L., G. De Belder, G. Schweitzer, M. Van der Auweraer and F.C. De Schryver, Femtosecond polarized transient absorption spectroscopy of a  $\text{C}_3$ -symmetric amino-substituted phenylbenzene derivative 295 (1998) 11
- Lau, A., see Pfeiffer, M. 295 (1998) 56
- Laurent, Ch., see Flahaut, E. 300 (1999) 236
- Lawley, K.P., see O'Keeffe, P. 298 (1998) 368
- Lawrance, W.D., see Alexander, U.N. 299 (1999) 291
- Laws, D.D., see Haake, M. 292 (1998) 686
- Lazaridis, M., Steady-state homogeneous nucleation of the sulfuric acid-water system 296 (1998) 477
- Lazzarini, E., The Smoluchowski equation for positronium atom reactions 293 (1998) 135
- Leach, M.O., see Wolber, J. 296 (1998) 391
- Leahy, D.J., see Osborn, D.L. 292 (1998) 651
- Leclerc, M., see DiCésare, N. 291 (1998) 487
- Le Coat, Y., R. Azria, M. Tronc, O. Ingólfsson and E. Illenberger, Medium enhanced, electron stimulated desorption of  $\text{CF}_3^-$  from condensed  $\text{CF}_3\text{I}$  296 (1998) 208
- Lecomte, C., see Espinosa, E. 300 (1999) 745
- Ledingham, K.W.D., see Singhal, R.P. 292 (1998) 643
- Lee, A.M., Investigations of the CASE approximation using the optimal partition of the Coulomb operator 292 (1998) 172
- Lee, B., see Kim, K.-H. 297 (1998) 65
- Lee, C.S., see Wang, N. 299 (1999) 237
- Lee, E.P.F., P. Soldán and T.G. Wright, The heat of formation of  $\text{NaO}^+(\text{X } ^3\Sigma^-)$  and  $\text{NaO}(\text{X } ^2\Pi)$  295 (1998) 354
- Lee, G.H., S.H. Huh, Y.C. Park, F. Hayakawa, Y. Negishi, A. Nakajima and K. Kaya, Photoelectron spectra of small nanophase W metal cluster anions 299 (1999) 309



- Lee, H.-S., Y.-K. Han, M.C. Kim, C. Bae and Y.S. Lee, Spin-orbit effects calculated by two-component coupled-cluster methods: test calculations on AuH, Au<sub>2</sub>, TiH and Ti<sub>2</sub> 293 (1998) 97
- Lee, H.W., see Kang, H. 292 (1998) 213
- Lee, M.-Z., see Chou, P.-T. 299 (1999) 327
- Lee, S., see Kim, K.-H. 297 (1998) 65
- Lee, S.H., P.T. Cummings, J.M. Simonson and R.E. Mesmer, Molecular dynamics simulation of the limiting conductance of NaCl in supercritical water 293 (1998) 289
- Lee, S.M., see Kang, H. 292 (1998) 213
- Lee, S.T., see Wang, N. 299 (1999) 237
- Lee, T.R., see Westcott, S.L. 300 (1999) 651
- Lee, Y.-P., see Kumar, A. 297 (1998) 300
- Lee, Y.-Y., see Kumar, A. 297 (1998) 300
- Lee, Y.G., see Loo, B.H. 297 (1998) 83
- Lee, Y.S., see Lee, H.-S. 293 (1998) 97
- Legon, A.C., see Cooke, S.A. 291 (1998) 269
- Legon, A.C., see Cooke, S.A. 298 (1998) 151
- Legon, A.C., see Wacławik, E.R. 295 (1998) 289
- Lehmann, K.K., see Bucher, C.R. 294 (1998) 173
- Lehn, J.-M., see Owrutsky, J.C. 293 (1998) 555
- Lehnert, A., see Härle, H. 293 (1998) 26
- Lei, J.-H., see Ren, H.-L. 292 (1998) 317
- Leicknam, J.-Cl., see Bratos, S. 291 (1998) 496
- Lemes, N.H.T., J.P. Braga and J.C. Belchior, Spherical potential energy function from second virial coefficient using Tikhonov regularization and truncated singular value decomposition 296 (1998) 233
- Lenchenkov, V.A., see Kloepfer, J.A. 298 (1998) 120
- Lendvay, G. and I. Mayer, Some difficulties in computing BSSE-corrected potential surfaces of chemical reactions 297 (1998) 365
- León, S., Ab initio G2(MP2,SVP) study of the reaction of hydroxymethylene with formaldehyde 296 (1998) 292
- Leś, A., see Borowicz, P. 291 (1998) 351
- Lesclaux, R., see Loison, J.C. 296 (1998) 350
- Lester, M.I., see Krause, P.J. 294 (1998) 518
- Létard, J.-F., see Ksenofontov, V. 294 (1998) 545
- Leutwyler, S., see Bach, A. 299 (1999) 381
- Levanon, H., see Shuali, Z. 300 (1999) 687
- Levchenko, G., see Ksenofontov, V. 294 (1998) 545
- Levin, Y., see Kuhn, P.S. 298 (1998) 51
- Levine, R.D., see Kornweitz, H. 294 (1998) 153
- Levine, R.D., see Remacle, F. 291 (1998) 453
- Levinger, N.E., see Pant, D. 292 (1998) 200
- Levit, C. and J. Sarfatti, Reply to Comment by I.P. Hamilton on: "Are the Bader Laplacian and the Bohm quantum potential equivalent?" 297 (1998) 263
- Levitt, M.H., see Edén, M. 293 (1998) 173
- Levy, M., see Nagy, Á. 296 (1998) 313
- Lewen, F., see Linnartz, H. 292 (1998) 188
- Ley, L., see Loison, J.C. 296 (1998) 350
- Li, B.-G., see Gao, X.-C. 297 (1998) 530

- Li, F., see Fan, L. 294 (1998) 443
- Li, G.-S., M.T.C. Martins-Costa, C. Millot and M.F. Ruiz-López, AM1/TIP3P molecular dynamics simulation of imidazole proton-relay processes in aqueous solution 297 (1998) 38
- Li, H., K.J. Franks and W. Kong, Photodissociation of ICN in a brute-force field: detection of the ( $I^* \ ^2P_{1/2}$ ) product 300 (1999) 247
- Li, J.-S. and K. Nishioka, Steady state nucleation-flux profile in binary systems 295 (1998) 211
- Li, L., T. He, X. Wang and F.-C. Liu, Laser-induced ESR shift of a paramagnetic transition metal complex ion  $[IrBr_6]^{2-}$  291 (1998) 179
- Li, S.-M., see Yu, Y.-X. 296 (1998) 131
- Li, Y., see Fan, L. 294 (1998) 443
- Li, Y., see Fan, L. 294 (1998) 443
- Li, Z.-S., see Yu, Y.-X. 296 (1998) 131
- Lian, L.-Y., see Norwood, T.J. 300 (1999) 429
- Liang, E.J., see Loo, B.H. 297 (1998) 83
- Liao, M., see Tan, H. 297 (1998) 173
- Liao, M.Z., see Feng, P.Y. 296 (1998) 283
- Li Bassi, A., see Barborini, E. 300 (1999) 633
- Licciardello, A., see Pignataro, B. 299 (1999) 430
- Lifshitz, E., A. Kaplan, E. Ehrenfreund and D. Meissner, Optically detected magnetic resonance as a tool to study the morphology of perylene-derivative thin film 300 (1999) 626
- Lifshitz, E., I.D. Litvin, H. Porteanu and A.A. Lipovskii, Magneto-optical properties of CdS nanoparticles embedded in phosphate glass 295 (1998) 249
- Liguori, L., see Asaro, F. 300 (1999) 414
- Lima, J.C., I. Abreu, R. Brouillard and A.L. Maçanita, Kinetics of ultra-fast excited state proton transfer from 7-hydroxy-4-methylflavylium chloride to water 298 (1998) 189
- Lin, C.-E., see Tsai, C.-S. 295 (1998) 509
- Lin, J.-C., see Tsai, C.-S. 295 (1998) 509
- Lin, M.C., see Kristyan, S. 297 (1998) 200
- Linden, N., H. Barjat and R. Freeman, An implementation of the Deutsch-Jozsa algorithm on a three-qubit NMR quantum computer 296 (1998) 61
- Linderberg, J., see Shehadi, I.A. 291 (1998) 325
- Lindh, R., see Nakayama, K. 300 (1999) 303
- Lindroos, M., see Seyller, Th. 291 (1998) 567
- Linnartz, H., T. Motylewski, F. Maiwald, D.A. Roth, F. Lewen, I. Pak and G. Winnewisser, Millimeter wave spectroscopy in a pulsed supersonic slit nozzle discharge 292 (1998) 188
- Linnertz, H., see Konopasek, I. 293 (1998) 429
- Lipiński, J., see Bartkowiak, W. 292 (1998) 92
- Lipovskii, A.A., see Lifshitz, E. 295 (1998) 249
- Lischka, H., see Müller, T. 293 (1998) 72
- Litvin, I.D., see Lifshitz, E. 295 (1998) 249
- Liu, C.-W., see Fan, H.-J. 300 (1999) 351
- Liu, F.-C., see Li, L. 291 (1998) 179
- Liu, F.-Q., see Gao, X.-C. 297 (1998) 530
- Liu, K., A. Kolessov, J.W. Partin, I. Bezel and C. Wittig, Probing the Cl-HCl complex via bond-specific photodissociation of  $(HCl)_2$  299 (1999) 374
- Liu, K., see Cruzan, J.D. 292 (1998) 667
- Liu, R.S., see Chen, J.M. 294 (1998) 209
- Liu, Y., Y. Wang and R.O. Claus, Layer-by-layer ionic self-assembly of Au colloids into multilayer thin-films with bulk metal conductivity 298 (1998) 315

- Liu, Y., see Zhou, S. 297 (1998) 77
- Liu, Z., R.J. Livingstone and P.B. Davies, Pulse pyrolysis infrared laser jet spectroscopy of free radicals 291 (1998) 480
- Liu, Z., see Fan, W.Y. 298 (1998) 222
- Livingstone, R.J., see Liu, Z. 291 (1998) 480
- Lo, D., see Lam, S.K. 297 (1998) 329
- Lo, K.K.-W., see Wang, C.-R. 296 (1998) 505
- Lobban, C., see Bowron, D.T. 293 (1998) 33
- Loffreda, D., D. Simon and P. Sautet, Vibrational frequency and chemisorption site: a DFT-periodic study of NO on Pd (111) and Rh (111) surfaces 291 (1998) 15
- Löhr, F., see Karimi-Nejad, Y. 300 (1999) 706
- Loison, J.C., L. Ley and R. Lesclaux, Kinetic study of OH radical reactions with chlorobutane isomers at 298 K 296 (1998) 350
- Longo, E., see Sambrano, J.R. 294 (1998) 1
- Loo, B.H., Y.G. Lee, E.J. Liang and W. Kiefer, Surface-enhanced Raman scattering from ferrocyanide and ferricyanide ions adsorbed on silver and copper colloids 297 (1998) 83
- López, G.E., see Ortiz, W. 298 (1998) 66
- Lopez, N., G. Pacchioni, F. Maseras and F. Illas, Hybrid quantum-mechanical and molecular mechanics study of Cu atoms deposition on SiO<sub>2</sub> surface defects 294 (1998) 611
- Lorenz, M., J. Agreiter, N. Caspary and V.E. Bondybey, Relaxation and vibrational fluorescence of WO in solid neon 291 (1998) 291
- Lou, L., see Zhang, W. 292 (1998) 133
- Lou, N.-Q., see Zhang, H. 300 (1999) 483
- Lounila, J., see Ruud, K. 297 (1998) 467
- Lounila, J., see Vaara, J. 296 (1998) 541
- Lowther, J.E., see Andriotis, A.N. 292 (1998) 487
- Lu, X., X. Xu, N. Wang and Q. Zhang, A quantum chemical study of the NO/MgO chemisorption system: hybrid B3LYP calculations on NO/(MgO)<sub>n</sub> (n = 4,6,8) model systems 300 (1999) 109
- Lü, X., X. Xu, N. Wang, Q. Zhang, M. Ehara and H. Nakatsuji, Cluster modeling of metal oxides: how to cut out a cluster? 291 (1998) 445
- Lü, X., see Xu, X. 292 (1998) 282
- Lucas, D.D., see Cruzan, J.D. 292 (1998) 667
- Lucas, J.M., see Romero, T. 292 (1998) 323
- Luckhaus, D., see Fehrensens, B. 300 (1999) 312
- Lüder, Ch. and K.H. Meiwes-Broer, Electron detachment energies of Pb<sub>N</sub><sup>-</sup> (N = 24-204) determined in a simple magnetic bottle photoelectron spectrometer 294 (1998) 391
- Lunell, S., see Wang, P. 292 (1998) 110
- Luo, J., see Hua, D. 299 (1999) 345
- Luo, Y., see Norman, P. 296 (1998) 8
- Lützenkirchen, K., see Rousseau, R. 295 (1998) 41
- Luz, Z., see Tekely, P. 291 (1998) 471
- Lyubovskaya, R.N., see Semkin, V.N. 295 (1998) 266
- Ma, B., see Kirschner, K.N. 295 (1998) 204
- Ma, C., see He, J. 295 (1998) 535
- Ma, N.L., How strong is the Ag<sup>+</sup>-ligand bond? 297 (1998) 230



- Ma, Y.-Z., J. Aschenbrücker, M. Miller and T. Gillbro, Ground-state vibrational coherence in chlorosomes of the green sulfur photosynthetic bacterium *Chlorobium phaeobacteroides* 300 (1999) 465
- Maçanita, A.L., see Lima, J.C. 298 (1998) 189
- Maccato, C., see Casarin, M. 300 (1999) 403
- Mackie, J.C., see Bacskay, G.B. 300 (1999) 321
- Madden, P., see Domene, C. 299 (1999) 51
- Madden, T.J., see Herbelin, J.M. 299 (1999) 583
- Mae, S., see Fukazawa, H. 294 (1998) 554
- Maeda, K., see Era, M. 296 (1998) 417
- Maeda, K., see Nakatsuji, S. 296 (1998) 159
- Mafé, S., P. Ramírez and A. Alcaraz, Electric field-assisted proton transfer and water dissociation at the junction of a fixed-charge bipolar membrane 294 (1998) 406
- Magnasco, V., M. Ottonelli, G. Figari, M. Rui and C. Costa, Long-range induction coefficients for like centrosymmetric linear molecules and an application to  $H_2-H_2$  291 (1998) 529
- Mahalakshmi, S. and M.K. Mishra, The  $^2B_1$  shape resonance in electron-formaldehyde scattering: an investigation using the dilated electron propagator method 296 (1998) 43
- Mahapatra, U.S., B. Datta and D. Mukherjee, Development of a size-consistent state-specific multireference perturbation theory with relaxed model-space coefficients 299 (1999) 42
- Maier, J.P., see Dopfer, O. 296 (1998) 585
- Maity, D.K., see Mohan, H. 300 (1999) 493
- Maiwald, F., see Linnartz, H. 292 (1998) 188
- Makarewicz, J., see Ha, T.-K. 299 (1999) 637
- Makarov, V.I., see Ishchenko, V.N. 299 (1999) 227
- Makri, N. and K. Thompson, Semiclassical influence functionals for quantum systems in anharmonic environments 291 (1998) 101
- Maksić, Z.B., see Kovačević, B. 293 (1998) 245
- Małecki, J.A., Study of self-association of 2-methyl-2-butanol based on non-linear dielectric effect 297 (1998) 29
- Malkin, V.G., see Malkina, O.L. 296 (1998) 93
- Malkina, O.L., B. Schimmelpfennig, M. Kaupp, B.A. Hess, P. Chandra, U. Wahlgren and V.G. Malkin, Spin-orbit corrections to NMR shielding constants from density functional theory. How important are the two-electron terms? 296 (1998) 93
- Malliaras, G.G., see Scott, J.C. 299 (1999) 115
- Malrieu, J.-P., see Pérez-Casany, M.P. 295 (1998) 181
- Malrieu, J.P., see Miguel, B. 294 (1998) 49
- Manaa, M.R. and C.F. Chabalowski, A theoretical treatment of the intersystem crossing in the spin-forbidden reaction  $NO(X^2\Pi) + CO(X^1\Sigma^+) \rightarrow N(^4S) + CO_2(X^1\Sigma_g^+)$  300 (1999) 619
- Manby, F.R. and P.J. Knowles, A perturbation theory using a local potential from Hartree-Fock orbitals 296 (1998) 1
- Mancera, R.L., Does salt increase the magnitude of the hydrophobic effect? A computer simulation study 296 (1998) 459
- Maniette, Y., see Maser, W.K. 292 (1998) 587
- Manke II, G.C., see Herbelin, J.M. 299 (1999) 583
- Manogaran, S., see Chakraborty, D. 294 (1998) 56
- Manoharan, M., On understanding the unique role of electrophilicity on  $C_{60}$  reactivity and strain on exothermicity in Diels-Alder and epoxidation reactions 296 (1998) 429
- Manoharan, P.T., see Gopinath, C.S. 296 (1998) 566

- Manthe, U., see Gerdt, T. 295 (1998) 167
- March, N.H., T. Gál and Á. Nagy, Differential equation for the ground-state electron density in a Hookean atom with two electrons repelling coulombically 292 (1998) 384
- Marchettini, N., see Rustici, M. 293 (1998) 145
- Marcus, A.H., see Tam, M.C.-M. 294 (1998) 217
- Marder, S.R., see Kogej, T. 298 (1998) 1
- Margrave, J.L., see Mickelson, E.T. 296 (1998) 188
- Märk, T.D., see Brüning, F. 292 (1998) 177
- Markgraber, D. and G. Engelhardt, <sup>39</sup>K MAS NMR of KNiF<sub>3</sub>: unexpected spin density at the potassium and first MAS NMR experiments in the antiferromagnetic state 300 (1999) 701
- Markovitsi, D., see Lampre, I. 293 (1998) 423
- Maroncelli, M., see Mente, S. 293 (1998) 515
- Maroun, F., F. Ozanam and J.-N. Chazalviel, In situ infrared monitoring of electrochemical adsorption/desorption of hydrogen on germanium 292 (1998) 493
- Marsden, C.J., see Ismail, N. 300 (1999) 296
- Marshall, P., see Yuan, J. 297 (1998) 553
- Martin, J., see Rudert, A.D. 294 (1998) 381
- Martin, J.M.L., Spectroscopic quality ab initio potential curves for CH, NH, OH and HF. A convergence study 292 (1998) 411
- Martínez, A., P. Calaminici, A.M. Köster and S.A. Mitchell, Interaction of Cr and Cr<sup>+</sup> with NO: a density functional study 299 (1999) 630
- Martínez, M.T., see Aoiz, F.J. 299 (1999) 25
- Martínez, M.T., see Maser, W.K. 292 (1998) 587
- Martínez, T.J., see Ben-Nun, M. 298 (1998) 57
- Martínez Ataz, E., see García-Ochoa, I. 296 (1998) 335
- Martinho, J.M.G., see Bodunov, E.N. 297 (1998) 419
- Martini, M., F. Meinardi and A. Scacco, Impurity-induced thermally stimulated luminescence of KMgF<sub>3</sub>:Ce<sup>3+</sup> crystals 293 (1998) 43
- Martins-Costa, M.T.C., see Li, G.-S. 297 (1998) 38
- Martoprawiro, M., see Bacskey, G.B. 300 (1999) 321
- Maruyama, Y. and Y. Tanimura, Pump-probe spectra and nuclear dynamics for a dissipative molecular system in a strong laser field: predissociation dynamics 292 (1998) 28
- Marx, D., see Rousseau, R. 295 (1998) 41
- Mase, K., see Nagasono, M. 298 (1998) 141
- Maser, W.K., E. Muñoz, A.M. Benito, M.T. Martínez, G.F. de la Fuente, Y. Maniette, E. Anglaret and J.-L. Sauvajol, Production of high-density single-walled nanotube material by a simple laser-ablation method 292 (1998) 587
- Maseras, F., see Lopez, N. 294 (1998) 611
- Mashiko, S., see Yanagi, H. 292 (1998) 332
- Masuhara, H., see Hatanaka, K. 300 (1999) 727
- Masuhara, H., see Yoshikawa, H. 293 (1998) 185
- Masumoto, K., see Ohtsuki, T. 300 (1999) 661
- Masuya, M., see Okamoto, Y. 299 (1999) 17
- Matejcik, S., see Brüning, F. 292 (1998) 177
- Mathur, D., see Kumar, G.R. 292 (1998) 647
- Matsui, E., see Ohkata, Y. 295 (1998) 17
- Matsumoto, A., see Tanaka, H. 293 (1998) 541
- Matsumoto, T., see Guan, W. 291 (1998) 161

- Matsumoto, Y., see Moriwaki, K. 292 (1998) 500
- Matsunaga, E., see Umemoto, H. 296 (1998) 203
- Matsuoka, H., see Yamaoka, H. 295 (1998) 245
- Matsushima, K., see Noda, M. 296 (1998) 599
- Matsushima, R., see Tokumura, K. 295 (1998) 516
- Matsushima, T., see Cao, G. 294 (1998) 419
- Matsuyama, H. and T. Koga, Electron-pair densities of singly charged atoms 300 (1999) 515
- Mattar, S.M., Calculation of the  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{14}\text{N}$  and  $^{33}\text{S}$  hyperfine tensors of the 1,3,2-dithiazol-2-yl radical using hybrid density functionals 300 (1999) 545
- Matveev, A.V., K. M. Neyman, G. Pacchioni and N. Rösch, Density functional study of  $\text{M}_4$  clusters ( $\text{M} = \text{Cu}, \text{Ag}, \text{Ni}, \text{Pd}$ ) deposited on the regular  $\text{MgO}(001)$  surface 299 (1999) 603
- Maus, M., W. Rettig, S. Depaemelaere, A. Onkelinx, F.C. De Schryver and K. Iwai, Solvent- and conformation-dependent electron transfer interactions in flexible biaromatic compounds: the case of 9-(dimethylanilino) phenanthrene 292 (1998) 115
- May, V., see Petrov, E.G. 294 (1998) 19
- May, V., see Schirrmeister, D.H. 297 (1998) 383
- Mayer, I., G. Räther and S. Suhai, Wannier-type orbitals derived from Mulliken's population analysis 293 (1998) 81
- Mayer, I., see Lendvay, G. 297 (1998) 365
- Mayer, M., see Pacchioni, G. 299 (1999) 137
- Mazumdar, C., see Hu, Z. 297 (1998) 321
- Mazzanti, L., see Konopasek, I. 293 (1998) 429
- Mazzavillani, A., see Dore, L. 300 (1999) 489
- Mazziotti, D.A., Spectral difference methods for solving differential equations 299 (1999) 473
- McCallum, R.W., see Chen, J.M. 294 (1998) 209
- McCanny, T., see Singhal, R.P. 292 (1998) 643
- McCormack, D.A. and G.-J. Kroes, Accuracy of trajectory methods for activated adsorption of  $\text{H}_2$  on  $\text{Cu}(100)$  296 (1998) 515
- McCourt, F.R.W., see Naumkin, F.Y. 292 (1998) 63
- McCourt, F.R.W., see Naumkin, F.Y. 294 (1998) 71
- McCoy, A.B., Comparison of self-consistent field treatments of kinetic couplings in calculations on polyatomic molecules 293 (1998) 103
- McElvany, S.W., see Garland, N.L. 297 (1998) 147
- McFadyen, G.G., see Andrews, D.P. 293 (1998) 343
- Mchedlov-Petrosyan, N.O., see Andrievsky, G.V. 300 (1999) 392
- McIlroy, A., Direct measurement of  $^1\text{CH}_2$  in flames by cavity ringdown laser absorption spectroscopy 296 (1998) 151
- McMullen, C.D., see Peric, M. 299 (1999) 69
- Meider, H. and M. Springborg, Constrained density-functional calculations for delocalized electrons: Hubbard parameters for polyacetylene 300 (1999) 339
- Meier, R., E. Weschke, A. Bievetski, C. Schüßler-Langeheine, Z. Hu and G. Kaindl, On the existence of monoxides on close-packed surfaces of lanthanide metals 292 (1998) 507
- Meijer, A.J.H.M., E.M. Goldfield, S.K. Gray and G.G. Balint-Kurti, Flux analysis for calculating reaction probabilities with real wave packets 293 (1998) 270
- Meijer, G., see von Helden, G. 299 (1999) 171
- Meinardi, F., see Martini, M. 293 (1998) 43
- Meissner, D., see Lifshitz, E. 300 (1999) 626
- Meissner, L. and I. Grabowski, A coupled-cluster correction to the multi-reference configuration interaction method 300 (1999) 53



- Meiwes-Broer, K.H., see Lüder, Ch. 294 (1998) 391
- Melandri, S., see Caminati, W. 294 (1998) 377
- Mele, F., N. Russo and F. Illas, Theoretical study of the interaction of alkali-metal atoms with CO<sub>2</sub> 295 (1998) 409
- Meleshko, V., Yu. Morokov and V. Schweigert, Structure of small hydrogenated silicon clusters: global search of low-energy states 300 (1999) 118
- Menéndez, M., see Aoiz, F.J. 299 (1999) 25
- Menon, M., see Andriotis, A.N. 292 (1998) 487
- Mente, S., S.J.V. Frankland, L. Reynolds and M. Maroncelli, Evaluation of classical potential functions for hydrogen bonding in 7-azaindole and 1-azacarbazole complexes 293 (1998) 515
- Menzel, R. and E. Thiel, Intersystem crossing rate constants of rhodamine dyes: influence of the amino-group substitution 291 (1998) 237
- Merchán, M., see Serrano-Andrés, L. 295 (1998) 195
- Mercier, X., E. Therssen, J.F. Pauwels and P. Desgroux, Cavity ring-down measurements of OH radical in atmospheric premixed and diffusion flames. A comparison with laser-induced fluorescence and direct laser absorption 299 (1999) 75
- Mérianne, M.-F., see Bernath, P. 297 (1998) 293
- Mesmer, R.E., see Lee, S.H. 293 (1998) 289
- Metka, U., see Härle, H. 293 (1998) 26
- Metzler, R., J. Klafter, J. Jortner and M. Volk, Multiple time scales for dispersive kinetics in early events of peptide folding 293 (1998) 477
- Meyer, E., see Berger, R. 294 (1998) 363
- Meyer, G., see Bartels, L. 291 (1998) 573
- Meyer, G., see Bartels, L. 297 (1998) 287
- Meyer, H.-D., see Worth, G.A. 299 (1999) 451
- Meyer, W., see Krämer, H.-G. 299 (1999) 212
- Meyers, F., see Kogej, T. 298 (1998) 1
- Micha, D.A. and Z. Yi, Optical control of yields of CO photodesorbed from Cu(001) by chirped light pulses: density matrix theory and calculations 298 (1998) 250
- Michaelian, K., A symbiotic algorithm for finding the lowest energy isomers of large clusters and molecules 293 (1998) 202
- Michaut, C., see Dupuis, B. 300 (1999) 169
- Michel-Beyerle, M.-E., see Voityuk, A.A. 296 (1998) 269
- Mickelson, E.T., C.B. Huffman, A.G. Rinzler, R.E. Smalley, R.H. Hauge and J.L. Margrave, Fluorination of single-wall carbon nanotubes 296 (1998) 188
- Miguel, B., N. Guihéry, J.P. Malrieu and P. Wind, Study of infinite polyacetylene from a Heisenberg Hamiltonian: dimerization and lowest excitation energies 294 (1998) 49
- Mihailovic, D., see Mrzel, A. 298 (1998) 329
- Miki, E.-i., see Morioka, Y. 292 (1998) 625
- Mila, F., see van Oosten, A.B. 295 (1998) 359
- Milani, P., see Barborini, E. 300 (1999) 633
- Miles, L.A., see Arthur, N.L. 295 (1998) 531
- Millemaggi, A., see Caminati, W. 294 (1998) 377
- Miller, M., see Ma, Y.-Z. 300 (1999) 465
- Miller, T.A., see Adams, S.F. 295 (1998) 305
- Miller, W.H., see Skinner, D.E. 300 (1999) 20
- Millot, C., see Li, G.-S. 297 (1998) 38
- Milman, V., see Winkler, B. 293 (1998) 284

- Mil'nikov, G.V., C. Zhu, H. Nakamura and V.I. Osherov, Semiclassical treatment of resonances in the collinear O + HO exchange reaction 293 (1998) 448
- Min, Z., R. Quandt and R. Bersohn, Kinetic energies of hydrogen atoms photodissociated from alkyl radicals 296 (1998) 372
- Minaev, B., J. Vaara, K. Ruud, O. Vahtras and H. Ågren, Internuclear distance dependence of the spin-orbit coupling contributions to proton NMR chemical shifts 295 (1998) 455
- Minehardt, T.J. and R.E. Wyatt, Quasi-classical dynamics of benzene overtone relaxation on an ab initio force field: 30-mode models of energy flow and survival probability for CH( $v = 2$ ) 295 (1998) 373
- Mink, H.J. and H.-H. Schmidtke, Electronic band assignments of high- and low-spin Ni[R<sub>2</sub>P(NR)<sub>2</sub>]<sub>2</sub> 291 (1998) 202
- Mishima, O., see Canpolat, M. 294 (1998) 9
- Mishima, O., see Kanno, H. 293 (1998) 412
- Mishra, M.K., see Mahalakshmi, S. 296 (1998) 43
- Mishra, M.K., see Venkatnathan, A. 296 (1998) 223
- Misochko, E.Ya., A.V. Akimov and C.A. Wight, Addition reactions of translationally hot fluorine atoms as a probe of long-range migration in crystalline argon: F + CO 293 (1998) 547
- Mitani, Y., see Kubozono, Y. 298 (1998) 335
- Mitchell, D.J. and J.N.S. Evans, Improved heteronuclear decoupling in REDOR with the use of TPPM 292 (1998) 656
- Mitchell, S.A., see Martínez, A. 299 (1999) 630
- Mito, M., see Nakatsuji, S. 296 (1998) 159
- Mitsushima, K., see Saito, Y. 294 (1998) 593
- Mittal, J.P., see Mohan, H. 300 (1999) 493
- Miyagawa, N., see Saito, Y. 294 (1998) 593
- Miyajima, S., see Kuwahara, D. 291 (1998) 244
- Miyamae, T., see Hino, S. 300 (1999) 145
- Miyasaka, H., T. Moriyama, T. Ide and A. Itaya, Picosecond dichroism measurements of photoconductive poly(*N*-vinylcarbazole) solid films: temperature effect on the hole migration reaction 292 (1998) 339
- Miyazaki, T., see Komaguchi, K. 300 (1999) 257
- M. Neyman, K., see Matveev, A.V. 299 (1999) 603
- Moerner, W.E., see Grunnet-Jepsen, A. 291 (1998) 553
- Mohan, H., D.K. Maity, S. Chattopadhyay and J.P. Mittal, Transformation of OH-adduct of 1-chloro-4-iodobutane into intra-molecular radical cation in neutral aqueous solution 300 (1999) 493
- Mokrane, A., see Salvatella, L. 296 (1998) 239
- Molin, Yu.N., see Bagryansky, V.A. 295 (1998) 230
- Molin, Yu.N., see Sviridenko, F.B. 297 (1998) 343
- Molins, E., see Espinosa, E. 300 (1999) 745
- Møller, K.B. and A.H. Zewail, Corrigendum to: "Femtosecond dynamics of transition states: the classical saddle-point barrier reactions" [Chem. Phys. Lett. 295 (1998) 1] 296 (1998) 619
- Møller, K.B. and A.H. Zewail, Femtosecond dynamics of transition states: the classical saddle-point barrier reactions 295 (1998) 1
- Møller, S., K.B. Andersen, J. Spanget-Larsen and J. Waluk, Excited-state intramolecular proton transfer in anthralin. Quantum chemical calculations and fluorescence spectra 291 (1998) 51
- Monnerville, M. and B. Pouilly, First quantum investigation of the photodissociation of the Ar-HBr complex: three-dimensional time-dependent approach 294 (1998) 473
- Montgomery Jr., H.E., Two-electron wavefunctions. Fourteenth-order expectation values 294 (1998) 468

- Monticone, S., R. Tufeu and A.V. Kanaev, Spectroscopical characterization of  $\text{TiO}_2$  powders prepared from stable colloidal solutions 295 (1998) 237
- Moog, R.S., W.W. Davis, S.G. Ostrowski and G.L. Wilson, Solvent effects on electronic transitions in several coumarins 299 (1999) 265
- Mooney, D.A., F. Müller-Plathe and K. Kremer, Simulation studies for liquid phenol: properties evaluated and tested over a range of temperatures 294 (1998) 135
- Moore, P.B., X. Ji, H. Ahlborn and B. Space, An instantaneous normal mode theory of condensed phase absorption: the vibrational spectrum of condensed  $\text{CS}_2$  from boiling to freezing 296 (1998) 259
- Mordziński, A., see Sepioł, J. 296 (1998) 549
- Mordziński, A., see Vdovin, A. 296 (1998) 557
- Mori, K., see Taneda, K. 298 (1998) 293
- Morimoto, H., see Nakatsuji, S. 296 (1998) 159
- Morioka, Y., S. Takeda, H. Tomizawa and E.-i. Miki, Molecular vibrations and structure of the light-induced metastable state of  $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$  292 (1998) 625
- Moriwaki, K., Y. Matsumoto, M. Ikai and K.-i. Tanaka, Spatial distribution of  $\text{N}_2$ ,  $\text{O}_2$  and NO molecules desorbing from a  $[\text{p}(2 \times 1)\text{-O} + \text{p}(2 \times 3)\text{-N}]\text{Ag}(110)$  surface 292 (1998) 500
- Moriyama, T., see Miyasaka, H. 292 (1998) 339
- Morokov, Yu., see Meleshko, V. 300 (1999) 118
- Moscardó, F. and J.C. Sancho-García, Exchange and correlation Kohn–Sham functionals for the helium atom: locality and homogeneity 294 (1998) 314
- Motylewski, T., see Linnartz, H. 292 (1998) 188
- Mozaffari-Afshar, M., see Hill, T. 292 (1998) 524
- Mrzel, A., A. Omerzu, P. Umek, D. Mihailovic, Z. Jagličić and Z. Trontelj, Ferromagnetism in a cobaltocene-doped fullerene derivative below 19 K due to unpaired spins only on fullerene molecules 298 (1998) 329
- Múčka, V., see Nikl, M. 291 (1998) 300
- Muga, J.G., see Palao, J.P. 292 (1998) 1
- Muigg, D., see Brüning, F. 292 (1998) 177
- Mukai, K., see Jamali, J.B. 292 (1998) 661
- Mukamel, S., see Tretiak, S. 297 (1998) 357
- Mukherjee, D., see Mahapatra, U.S. 299 (1999) 42
- Müller, M., see van Oijen, A.M. 292 (1998) 183
- Müller-Plathe, F., see Mooney, D.A. 294 (1998) 135
- Müller, T., P. Dupré, P.H. Vaccaro, F. Pérez-Bernal, M. Ibrahim and F. Iachello, Algebraic approach for the calculation of polyatomic Franck–Condon factors. Application to the vibronically resolved emission spectrum of  $\text{S}_2\text{O}$  292 (1998) 243
- Müller, T., S.S. Xantheas, H. Dachsel, R.J. Harrison, J. Nieplocha, R. Shepard, G.S. Kedziora and H. Lischka, A systematic ab initio investigation of the open and ring structures of ozone 293 (1998) 72
- Muñoz, E., see Maser, W.K. 292 (1998) 587
- Munters, T., see Clays, K. 293 (1998) 337
- Murakami, Y., see Yoshida, Y. 291 (1998) 31
- Murga, L.F., see Shehadi, I.A. 291 (1998) 325
- Murgida, D.H., R. Erra Balsells, P.R. Crippa and C. Viappiani, Type I photosensitized reactions of oxopurines. Kinetics and thermodynamics of the reaction with triplet benzophenone by time-resolved photoacoustic spectroscopy 294 (1998) 538



- Murrell, J.N., see Bosanac, S.D. 291 (1998) 64  
Muthukumaran, R., see Gopinath, C.S. 296 (1998) 566
- Nabeshima, M., see Okamoto, Y. 299 (1999) 17  
Nachtigallová, D., see Slavíček, P. 300 (1999) 561  
Nadeem, A., see Baig, M.A. 296 (1998) 403  
Nagae, H., see Sashima, T. 299 (1999) 187  
Nagamura, T., S. Kashiwara and H. Kawai, First intramolecular charge resonance band observed at room temperature in solution by steady photolysis of 1,3-bis(4-(4-nitrophenyl)pyridinium)propane tetraphenylborate 294 (1998) 167  
Nagaosa, K., see Tokumura, K. 295 (1998) 516  
Någård, M.B. and J.B.C. Pettersson, Internal excitation of ethanol molecules emitted during cluster-surface collisions 293 (1998) 535  
Nagasono, M., K. Mase, S. Tanaka and T. Urisu, State-selected ion desorption from condensed H<sub>2</sub>O at 80 K studied by Auger electron-photoion coincidence spectroscopy 298 (1998) 141  
Nagata, T., see Tsukuda, T. 295 (1998) 416  
Nagels, B., P. Bakker, L.J.F. Hermans and P.L. Chapovsky, Violation of nuclear-spin symmetry in collisions of symmetric tops 294 (1998) 387  
Nagy, Á. and M. Levy, Tests for new ionization formula in density functional theory 296 (1998) 313  
Nagy, A., see Tóthová, M. 299 (1999) 243  
Nagy, Á., see Andrejkovics, I. 296 (1998) 489  
Nagy, Á., see March, N.H. 292 (1998) 384  
Nagy, J.B., see Ahlskog, M. 300 (1999) 202  
Nakabayashi, S., D.A. Tryk, A. Fujishima and N. Ohta, Electrochemical reduction of Cu<sup>2+</sup> without surface trapping on synthetic conductive diamond electrodes 300 (1999) 409  
Nakabayashi, S., I. Krastev, R. Aogaki and K. Inokuma, Electrochemical instability of Ag/Sb co-deposition coupled with a magnetohydrodynamic flow 294 (1998) 204  
Nakabayashi, T., see Kosugi, K. 291 (1998) 253  
Nakahara, H., see Sueki, K. 291 (1998) 37  
Nakahara, H., see Sueki, K. 300 (1999) 140  
Nakai, T., see Kuwahara, D. 291 (1998) 244  
Nakajima, A., see Lee, G.H. 299 (1999) 309  
Nakajima, A., see Negishi, Y. 294 (1998) 370  
Nakajima, H., see Kometani, N. 294 (1998) 619  
Nakajima, T. and H. Nakatsuji, Second-order perturbative approximation to the SAC/SAC-CI method 300 (1999) 1  
Nakamura, H. and S. Kato, Quantum calculation of the vibrational energy level structure of N<sub>2</sub>O based on ab initio potential surface 297 (1998) 187  
Nakamura, H., see Mil'nikov, G.V. 293 (1998) 448  
Nakano, H., see Choe, Y.-K. 295 (1998) 380  
Nakano, M. and K. Yamaguchi, Electron-photon field dynamics: a molecular aggregate interacting with an initially one-mode coherent photon field 295 (1998) 328  
Nakano, M. and K. Yamaguchi, Quasiprobability distribution dynamics of an initially one-mode coherent photon field interacting with two- and three-state molecular systems 295 (1998) 317  
Nakata, M., see Kudoh, S. 296 (1998) 329  
Nakatsuji, H., J. Hasegawa and K. Ohkawa, Excited states and electron transfer mechanism in the photosynthetic reaction center of *Rhodospseudomonas viridis*: SAC-CI study 296 (1998) 499  
Nakatsuji, H., see Honda, Y. 293 (1998) 230  
Nakatsuji, H., see Lü, X. 291 (1998) 445

- Nakatsuji, H., see Nakajima, T. 300 (1999) 1
- Nakatsuji, H., see Xu, X. 292 (1998) 282
- Nakatsuji, S., H. Morimoto, H. Anzai, J. Kawashima, K. Maeda, M. Mito and K. Takeda, Magnetic properties of 2,5-difluorophenyl- $\alpha$ -nitronyl nitroxide and related position isomers 296 (1998) 159
- Nakayama, K., K. Hirao and R. Lindh, Different bases for different correlation effects: multireference Møller-Plesset perturbation theory in the extended basis function space 300 (1999) 303
- Nakazawa, T., see Okamoto, Y. 299 (1999) 17
- Nanba, Y., see Kato, M. 294 (1998) 626
- Narayana Rao, D., see Venugopal Rao, S. 297 (1998) 491
- Natterer, J., T. Greve and J. Bargon, Orthodeuterium induced polarization 293 (1998) 455
- Naumkin, F.Y. and F.R.W. McCourt, Ab initio-based potential energy surfaces and predicted microwave spectra of the Ar-I<sub>2</sub>( $X^1\Sigma_g^+$ ) Van der Waals complex 294 (1998) 71
- Naumkin, F.Y. and F.R.W. McCourt, On the influence of rare gas atom-chlorine ion potentials on the ground state Rg-Cl<sub>2</sub> interactions 292 (1998) 63
- Neal, M.P. and A.J. Parker, Computer simulations using a longitudinal quadrupolar Gay-Berne model: effect of the quadrupole magnitude on the formation of the smectic phase 294 (1998) 277
- Nebot-Gil, I., see Anane, H. 296 (1998) 277
- Nebot-Gil, I., see Pérez-Casany, M.P. 295 (1998) 181
- Nebot-Gil, I., see Pitarch-Ruiz, J. 291 (1998) 407
- Nedeljković, J.M., see Čomor, M.I. 299 (1999) 233
- Nefedov, O.M., see Bagryansky, V.A. 295 (1998) 230
- Negishi, Y., H. Kawamata, F. Hayakawa, A. Nakajima and K. Kaya, The infrared HOMO-LUMO gap of germanium clusters 294 (1998) 370
- Negishi, Y., see Lee, G.H. 299 (1999) 309
- Nelson, H.H., see Owrutsky, J.C. 293 (1998) 555
- Nemukhin, A.V., see Grigorenko, B.L. 296 (1998) 84
- Nepijko, S., see Adelt, M. 291 (1998) 425
- Nešpůrek, S., see Sworakowski, J. 298 (1998) 21
- Neuhauser, D., see Anderson, S.M. 291 (1998) 387
- Neuhauser, D., see Wall, M.R. 291 (1998) 465
- Neuhauser, R., see Siglow, K. 293 (1998) 19
- Neumann, D.A., see Guerrero, H.M. 297 (1998) 265
- Neumark, D.M., see Asmis, K.R. 295 (1998) 75
- Neumark, D.M., see Osborn, D.L. 292 (1998) 651
- Neumark, D.M., see Taylor, T.R. 297 (1998) 133
- Neusser, H.J., see Siglow, K. 293 (1998) 19
- Neville, J.J., T. Tylliszczak, A.P. Hitchcock, A. Jürgensen and R.G. Cavell, P 1s spectroscopy of SPF<sub>3</sub>: spectral assignments aided by angle-resolved photodissociation 300 (1999) 451
- Newson, K.A. and S.D. Price, Intramolecular isotope effects in the bond-forming reaction of CF<sub>2</sub><sup>2+</sup> with HD 294 (1998) 223
- Nguyen, H.M.T., see Nguyen, M.T. 300 (1999) 346
- Nguyen, M.T. and H.M.T. Nguyen, On the heats of formation of methylketene, dimethylketene and related cations 300 (1999) 346
- Nguyen, M.T., S. Creve and T.-K. Ha, On the formation of the  $\cdot\text{CH}_2\text{CH}_2\text{CH}=\text{NH}_2^+$  distonic radical cation upon ionization of cyclopropylamine and allylamine 293 (1998) 90
- Niedner-Schatteburg, G., see Achatz, U. 291 (1998) 459

- Nielsen, N.Chr., see Larsen, F.H. 292 (1998) 467
- Nieplocha, J., see Müller, T. 293 (1998) 72
- Niikura, H. and S. Hirayama, Shift from an inverse to a normal isotope effect on the non-radiative decay rate of anthracene-d<sub>10</sub> observed under partially jet-cooled conditions 296 (1998) 343
- Nikl, M., P. Straková, K. Nitsch, V. Petříček, V. Múčka, O. Jarolímek, J. Novák and P. Fabeni, Energy transfer processes in PbWO<sub>4</sub> luminescence 291 (1998) 300
- Nikolaev, P., see Hafner, J.H. 296 (1998) 195
- Ning, C.-L., see Kennedy, G.R. 292 (1998) 161
- Nishi, N., see Kosugi, K. 291 (1998) 253
- Nishibori, E., M. Takata, M. Sakata, M. Inakuma and H. Shinohara, Determination of the cage structure of Sc@C<sub>82</sub> by synchrotron powder diffraction 298 (1998) 79
- Nishina, Y., see Saito, Y. 294 (1998) 593
- Nishina, Y., see Sugano, M. 292 (1998) 575
- Nishino, M., Y. Yoshioka and K. Yamaguchi, Effective exchange interactions and magnetic phase transition temperatures in Prussian blue analogs: a study by density functional theory 297 (1998) 51
- Nishino, Y., S. Yano, M. Tansho and T. Yamaguchi, Dynamic mechanical properties of strontium stearate 296 (1998) 408
- Nishioka, K., see Li, J.-S. 295 (1998) 211
- Nishiyama, H., see Saito, N. 297 (1998) 72
- Nitsch, K., see Nikl, M. 291 (1998) 300
- Nitta, T., see Takahashi, H. 294 (1998) 95
- Noda, M., K. Matsushima, K. Seki and M. Yagi, Effects of protonation on the lowest triplet state of *trans*-4,4'-dipyridylethylene. A time-resolved electron paramagnetic resonance study 296 (1998) 599
- Noga, J., see Svrček, M. 299 (1999) 151
- Noid, D.W., see Runge, K. 299 (1999) 352
- Nolen, S. and S.T. Ruggiero, Tunneling spectroscopy of fullerene/Ge multilayer systems 300 (1999) 656
- Nölle, A., C. Krumscheid and H. Heydtmann, Determination of quantum yields in the UV photolysis of COF<sub>2</sub> and COFCl 299 (1999) 561
- Nomoto, T., see Hirata, Y. 293 (1998) 371
- Norman, P., Y. Luo and H. Ågren, Structure-to-property relations for two-photon absorption of hydrocarbon oligomers 296 (1998) 8
- Norwood, T.J., M.L. Tillett and L.-Y. Lian, Influence of cross-correlation between the chemical shift anisotropies of pairs of nuclei on multiple-quantum relaxation rates in macromolecules 300 (1999) 429
- Novák, J., see Nikl, M. 291 (1998) 300
- Nowek, A., see Jabalameli, A. 295 (1998) 135
- Nyman, G., see Yu, H.-G. 298 (1998) 27
- Obsil, T., see Konopasek, I. 293 (1998) 429
- Ogi, Y. and K. Tsukiyama, Switching of the two competing amplified spontaneous emission channels in NO 296 (1998) 384
- O'Grady, W.E., see Ramaker, D.E. 299 (1999) 221
- Ogura, K., see Seko, T. 291 (1998) 438
- Ohanessian, G., see Gee, C. 298 (1998) 85
- Ohba, Y., see Fujisawa, J. 294 (1998) 248



- Ohkata, Y., T. Tsuno, E. Matsui, H. Takanashi and K. Itoh, A combined method of multiple-reflection and optical-wave-guide Raman scattering spectroscopies for studying the electric-field-induced reorientation of a ferroelectric liquid crystal cell 295 (1998) 17
- Ohkawa, K., see Nakatsuji, H. 296 (1998) 499
- Ohlsson, P.I., see Edholm, O. 291 (1998) 501
- Ohno, Y., see Cao, G. 294 (1998) 419
- Ohta, N., T. Kanada, I. Yamazaki and M. Itoh, External electric field effects on the fluorescence of methylene-linked pyrene and *N,N*-dimethylaniline doped in a PMMA polymer film 292 (1998) 535
- Ohta, N., see Nakabayashi, S. 300 (1999) 409
- Ohta, T., see Terada, S. 300 (1999) 645
- Ohta, Y., see Tokumura, K. 295 (1998) 516
- Ohtake, T., N. Sonoyama and T. Sakata, Electrochemical luminescence of  $\text{ZnGa}_2\text{O}_4$  and  $\text{ZnGa}_2\text{O}_4\text{:Mn}$  electrodes 298 (1998) 395
- Ohtani, H., M. Kaneko, M. Ishikawa, N. Kamiya and N. Yamamoto, Picosecond-millisecond dual-time-base spectroscopy of fluorescent photointermediates formed in the purple membrane of *Halobacterium halobium* 299 (1999) 571
- Ohtsuki, T., K. Masumoto, T. Tanaka and K. Komatsu, Formation of dimer, trimer, and tetramer of  $\text{C}_{60}$  and  $\text{C}_{70}$  by  $\gamma$ -ray, charged-particle irradiation, and their HPLC separation 300 (1999) 661
- Okada, K., see Hikida, T. 292 (1998) 638
- Okada, T., see Hirata, Y. 293 (1998) 371
- Okamoto, Y., M. Masuya, M. Nabeshima and T. Nakazawa,  $\beta$ -sheet formation in BPTI(16-36) by Monte Carlo simulated annealing 299 (1999) 17
- Okamoto, Y., see Hansmann, U.H.E. 297 (1998) 374
- Okamoto, Y., see Kinoshita, M. 297 (1998) 433
- Okawa, M., see Awaga, K. 293 (1998) 352
- Okazaki, S., see Shiga, M. 292 (1998) 431
- O'Keefe, A., Integrated cavity output analysis of ultra-weak absorption 293 (1998) 331
- O'Keefe, P., T. Ridley, S. Wang, K.P. Lawley and R.J. Donovan, Photodissociation of ozone between 335 and 352 nm to give  $\text{O}_2(\text{b}^1\Sigma_g^+) + \text{O}(^3\text{P}_j)$  298 (1998) 368
- Okumura, K. and Y. Tanimura, Two-dimensional THz spectroscopy of liquids: non-linear vibrational response to a series of THz laser pulses 295 (1998) 298
- Okutsu, T., T. Kageyama, N. Kounose, J. Tsuchiya and H. Hiratsuka, Phosphorescence spectra of bromobenzene in highly viscous glassy matrices 299 (1999) 597
- Olbrechts, G., see Clays, K. 293 (1998) 337
- Oldenburg, S.J., see Westcott, S.L. 300 (1999) 651
- Oleinikova, A. and M. Bonetti, Coexistence curve of the ionic binary mixture tetra-*n*-butylammonium picrate in 1-dodecanol 299 (1999) 417
- Oliva, M., V.S. Safont, J. Andr s and O. Tapia, Molecular mechanism for oxygenation pathway in Rubisco. Mapping transition structures and intermediates for model compounds of the substrate system 294 (1998) 87
- Olivucci, M., see Klein, S. 292 (1998) 259
- Olkhov, R.V., see Dopfer, O. 296 (1998) 585
- Olsen, J., see Coriani, S. 300 (1999) 61
- Olsen, J., see Larsen, H. 291 (1998) 536
- Olszewski, R., P. Woli ski and M. Zubek, Excitation of carbon monoxide by electron impact in the 8-17 eV energy range 297 (1998) 537

- O'Malley, P.J., A density functional study of the effect of orientation of hydrogen bond donation on the hyperfine couplings of benzosemiquinones: relevance to semiquinone-protein hydrogen bonding interactions in vivo 291 (1998) 367
- Omerzu, A., see Mrzel, A. 298 (1998) 329
- Omori, T., T. Suzuki and T. Ichimura, Study of intramolecular hydrogen abstraction on photoexcited 1,3-dimethylantrone in the condensed phase 293 (1998) 436
- Ondrechen, M.J., see Shehadi, I.A. 291 (1998) 325
- Onipko, A., An extension of the McConnell superexchange formula to the case of real conjugated oligomers 292 (1998) 267
- Onkelinx, A., see Maus, M. 292 (1998) 115
- Ono, M. and M. Kotani, Ionization of molecular excitons detected by electron emission: coronene and  $\alpha$ -perylene 295 (1998) 34
- Ono, M. and M. Kotani, Time-resolved measurement of excitonic electron emission from a fluoranthene crystal 295 (1998) 493
- Ono, T., see Hasegawa, K. 300 (1999) 9
- Oosterbeek, H., see Fukui, K. 299 (1999) 158
- Orbán, M., see Kurin-Csörgei, K. 295 (1998) 70
- Ordon, P. and L. Komorowski, Nuclear reactivity and nuclear stiffness in density functional theory 292 (1998) 22
- Oref, I., see Bernshtein, V. 300 (1999) 104
- Orlando, J.J., see Phillips, J.A. 296 (1998) 377
- Orlov, A.Yu., see Feldman, V.I. 300 (1999) 713
- Ornellas, F.R., Transition moment function, transition probabilities, and radiative lifetimes in the  $A^1\Pi-X^1\Sigma^+$  system of the CS molecule 296 (1998) 25
- Ortiz, J.V., Electron detachment energies of closed-shell anions calculated with a renormalized electron propagator 296 (1998) 494
- Ortiz, J.V., Single-reference electron propagator calculations on vertical ionization energies of ozone 297 (1998) 193
- Ortiz, W., A. Perlloni and G.E. López, Extending the J-walking Monte Carlo algorithm to the isothermal-isobaric ensemble: solid-liquid equilibrium in clusters 298 (1998) 66
- Osad'ko, I.S. and N.N. Zaitsev, Are there charged two-level systems in polymers? 293 (1998) 138
- Osborn, D.L., D.J. Leahy, E.H. Kim, E. de Beer and D.M. Neumark, Photoelectron spectroscopy of  $\text{CH}_3\text{O}^-$  and  $\text{CD}_3\text{O}^-$  292 (1998) 651
- Osherov, V.I., see Mil'nikov, G.V. 293 (1998) 448
- Oshima, I., see Fukui, K. 299 (1999) 158
- Ostrowski, S.G., see Moog, R.S. 299 (1999) 265
- Otomo, A., see Yanagi, H. 292 (1998) 332
- Otto, P., see Hu, A. 293 (1998) 277
- Ottonelli, M., see Magnasco, V. 291 (1998) 529
- Owrutsky, J.C., H.H. Nelson, A.P. Baronavski, O.-K. Kim, G.M. Tsivgoulis, S.L. Gilat and J.-M. Lehn, Optical properties and dynamics of a photochromic bisthiénylene in solution and in a polymer film 293 (1998) 555
- Ozanam, F., see Maroun, F. 292 (1998) 493
- Ozhegova, N.V., see Grigorenko, B.L. 296 (1998) 84
- Paa, W., J.-P. Yang, M. Helbig, J. Hein and S. Rentsch, Femtosecond time-resolved measurements of terthiophene: fast singlet-triplet intersystem crossing 292 (1998) 607

- Pacchioni, G., M. Mayer, S. Krüger and N. Rösch, Bonding and adsorbate core level shifts of transition metal atoms on the Al(100) surface from density functional calculations 299 (1999) 137
- Pacchioni, G., see Lopez, N. 294 (1998) 611
- Pacchioni, G., see Matveev, A.V. 299 (1999) 603
- Paddon-Row, M.N., see Scholes, G.D. 292 (1998) 601
- Padmanabhan, J., see Subramanian, V. 294 (1998) 285
- Pak, I., see Linnartz, H. 292 (1998) 188
- Pak, I., see Roth, D.A. 298 (1998) 381
- Pal, S., see Basu Kumar, A. 295 (1998) 189
- Pal, S., see Vaval, N. 300 (1999) 125
- Palao, J.P. and J.G. Muga, A simple construction procedure of absorbing potentials 292 (1998) 1
- Palmer, P.M. and M.R. Topp, Spectroscopic properties of jet-cooled methanol clusters ( $n = 1-6$ ) attached to anthracene 292 (1998) 307
- Palmer, P.M., see Pryor, B.A. 299 (1999) 536
- Palmer, R.E., see Thomas, P.J. 294 (1998) 229
- Palomar, J., see Catalán, J. 293 (1998) 511
- Pan, B.C., C.Z. Wang, D.E. Turner and K.M. Ho, Structures and properties of  $\text{Si}_{13}$  isomers 292 (1998) 75
- Pan, D., L.C.T. Shoute and D.L. Phillips, Nanosecond time-resolved resonance Raman investigation of the radical cation of 4,4'-dibromobiphenyl and the  $T_1 \rightarrow T_n$  transition of 4,4'-dibromobiphenyl 292 (1998) 677
- Pan, Z.W., S.S. Xie, B.H. Chang, L.F. Sun, W.Y. Zhou and G. Wang, Direct growth of aligned open carbon nanotubes by chemical vapor deposition 299 (1999) 97
- Pancheshnyi, S.V., S.M. Starikovskaia and A.Y. Starikovskii, Measurements of rate constants of the  $\text{N}_2(\text{C}^3\Pi_u, v' = 0)$  and  $\text{N}_2^+(\text{B}^2\Sigma_u^+, v' = 0)$  deactivation by  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{H}_2$ , CO and  $\text{H}_2\text{O}$  molecules in afterglow of the nanosecond discharge 294 (1998) 523
- Pang, W.N., R.C. Shang, J.F. Gao, N.F. Gao, X.J. Chen and M.S. Deleuze, Investigation of the valence electronic structure of  $n$ -butane using ( $e, 2e$ ) spectroscopy 296 (1998) 605
- Pang, W.N., R.C. Shang, N.F. Gao, W.X. Zhang, X.J. Chen, Y. Zheng and C.E. Brion, Measurements of the valence shell binding energy spectrum and momentum profiles of the frontier orbitals of propane by binary ( $e, 2e$ ) spectroscopy 299 (1999) 207
- Pant, D. and N.E. Levinger, Dynamics of polar solvation at the surface of a  $\text{ZrO}_2$  nanoparticle 292 (1998) 200
- Paolucci, G., see Polzonetti, G. 292 (1998) 515
- Park, J., Collisional excitation of  $\text{CO}_2(00^00)$  vibrationless state by the highly translationally excited HCN produced from the photodissociation of  $s$ -triazine 293 (1998) 383
- Park, J. and J.F. Hershberger, Kinetics of the  $\text{CN} + \text{OCS}$  reaction 295 (1998) 89
- Park, Y.C., see Lee, G.H. 299 (1999) 309
- Parker, A.J., see Neal, M.P. 294 (1998) 277
- Parker, D.H., see Bakker, B.L.G. 294 (1998) 565
- Parlett, L.C., Laser-induced ESR shifts in the sodium atom spectrum 296 (1998) 571
- Parnaíba-daSilva, A.J. and A.A.S. da Gama, Interference effects on through-bond electronic interaction propagation 296 (1998) 483
- Partin, J.W., see Liu, K. 299 (1999) 374
- Partridge, H., see Bauschlicher Jr., C.W. 300 (1999) 364
- Pashov, A., W. Jastrzębski and P. Kowalczyk, The  $\text{B}^1\Pi$  and  $\text{C}^1\Sigma^+$  states of  $\text{KLi}$  292 (1998) 615
- Patil, S.H. and K.T. Tang, A simple method for polarizabilities and hyperpolarizabilities of alkali isoelectronic systems 295 (1998) 152
- Patil, S.H., see Johann, C. 295 (1998) 158



- Pattard, T. and J.M. Rost, A route to chaos in classical atom-diatom collisions 291 (1998) 360
- Patterson, H.H., see Strasser, J. 295 (1998) 95
- Patzelt, H., see Weigend, F. 294 (1998) 143
- Paul, J., see Edholm, O. 291 (1998) 501
- Pauwels, J.F., see Mercier, X. 299 (1999) 75
- Pavese, M., D.R. Berard and G.A. Voth, Ab initio centroid molecular dynamics: a fully quantum method for condensed-phase dynamics simulations 300 (1999) 93
- Pavlov, M., see Siegbahn, P.E.M. 292 (1998) 421
- Pedersen, M.Ø., M.-L. Bocquet, P. Sautet, E. Lægsgaard, I. Stensgaard and F. Besenbacher, CO on Pt(111): binding site assignment from the interplay between measured and calculated STM images 299 (1999) 403
- Pedersen, T.B. and H. Koch, Gauge invariance of the coupled cluster oscillator strength 293 (1998) 251
- Pedulla, J.M., K. Kim and K.D. Jordan, Theoretical study of the  $n$ -body interaction energies of the ring, cage and prism forms of  $(\text{H}_2\text{O})_6$  291 (1998) 78
- Peel, J.B., see Khairallah, G. 296 (1998) 545
- Peigney, A., see Flahaut, E. 300 (1999) 236
- Pekker, S., see Kamarás, K. 295 (1998) 279
- Pelikán, P., see Svrček, M. 299 (1999) 151
- Pellizer, G., see Asaro, F. 300 (1999) 414
- Peluso, A., see Del Re, G. 299 (1999) 511
- Peng, W.X., see Singhal, R.P. 292 (1998) 643
- Pénicaud, A., see Taylor, R. 295 (1998) 481
- Pérez-Bernal, F., see Müller, T. 292 (1998) 243
- Pérez-Casany, M.P., I. Nebot-Gil, J. Sánchez-Marín, O. Castell Marcos and J.-P. Malrieu, Vertical spectrum of ethene: uncontracted versus contracted correlation methods and the role of the adapted molecular orbitals 295 (1998) 181
- Pérez, P. and R. Contreras, A theoretical analysis of the gas-phase protonation of hydroxylamine, methyl-derivatives and aliphatic amino acids 293 (1998) 239
- Periasamy, N., see Krishna, M.M.G. 298 (1998) 359
- Peric, M., C.D. McMullen, V. Andrade and B.L. Bales, A novel two microwave field ESR implemented by double field modulation 299 (1999) 69
- Perlloni, A., see Ortiz, W. 298 (1998) 66
- Pernpointner, M. and P. Schwerdtfeger, Accurate nuclear quadrupole moments of the gallium isotopes  $^{69}\text{Ga}$  and  $^{71}\text{Ga}$  within the PCNQM model 295 (1998) 347
- Perry, J.W., see Kogej, T. 298 (1998) 1
- Persky, A., Kinetics of the reactions  $\text{F} + \text{H}_2\text{S}$  and  $\text{F} + \text{D}_2\text{S}$  at 298 K 298 (1998) 390
- Persoons, A., see Clays, K. 293 (1998) 337
- Pesch, T.C., see Allen, M.D. 293 (1998) 397
- Peteanu, L., see Premvardhan, L. 296 (1998) 521
- Pethica, J.B., see Wee, A.T.S. 298 (1998) 146
- Petrella, G., L. Cassidei and F. Ciriaco, He scattering from disordered surfaces: specular intensity, cross-section and surface structure 291 (1998) 562
- Petříček, V., see Nikl, M. 291 (1998) 300
- Petrov, E.G., I.S. Tolokh and V. May, Blocking of bridge-mediated electron transfer by an external magnetic field 294 (1998) 19
- Pettersson, J.B.C., see Någård, M.B. 293 (1998) 535
- Pettinger, B., see Bilger, C. 294 (1998) 425
- Pfab, J., see Kennedy, G.R. 292 (1998) 161

- Pfänder, N., see Kuhlmann, U. 294 (1998) 237
- Pfeiffer, M., W. Werncke, S. Hogiu, A. Kummrow and A. Lau, Strong vibronic coupling in the first excited singlet state of diphenylhexatriene by an asymmetric low-frequency mode 295 (1998) 56
- Pfeiffer, T., O. Forberich and F.J. Comes, Tropospheric OH formation by ozonolysis of terpenes 298 (1998) 351
- Phillips, D.L., see Pan, D. 292 (1998) 677
- Phillips, D.L., see Zheng, X. 292 (1998) 295
- Phillips, D.L., see Zheng, X. 296 (1998) 173
- Phillips, J.A., J.J. Orlando, G.S. Tyndall and V. Vaida, Integrated intensities of OH vibrational overtones in alcohols 296 (1998) 377
- Phillips, L.F., Theoretical cross-sections for resonant exchange of rotational energy in a Stark field 291 (1998) 94
- Piel, J., see Wurzer, A.J. 299 (1999) 296
- Piet, J.J., see Scholes, G.D. 292 (1998) 601
- Pignataro, B., C. Consalvo, G. Compagnini and A. Licciardello, Barium stearate Langmuir-Blodgett films investigated by mapping adhesion forces with atomic force microscopy 299 (1999) 430
- Pin, S., see Haouz, A. 294 (1998) 197
- Pines, A., see Haake, M. 292 (1998) 686
- Pingel, U.-T., J.-P. Amoureux, T. Anupold, F. Bauer, H. Ernst, C. Fernandez, D. Freude and A. Samoson, High-field  $^{17}\text{O}$  NMR studies of the SiOAl bond in solids 294 (1998) 345
- Pinkerton, T.D., see Scovell, D.L. 294 (1998) 255
- Pinsky, M., see Keinan, S. 298 (1998) 43
- Piper, L.G., Experimental determination of the Einstein coefficient for the  $\text{N}(^2\text{P}-^4\text{S})$  transition 296 (1998) 397
- Piseri, P., see Barborini, E. 300 (1999) 633
- Pitarch-Ruiz, J., J. Sánchez-Marín, I. Nebot-Gil and N.B. Amor, Application of the size-consistent self-consistent intermediate hamiltonian approach to different SDCI. The excited states of  $\text{N}_2$  291 (1998) 407
- Pizzoferrato, R., see Casalboni, M. 291 (1998) 167
- Plato, M., see Keinan, S. 298 (1998) 43
- Platz, T. and W. Demtröder, Sub-Doppler optothermal overtone spectroscopy of ethylene and dichloroethylene 294 (1998) 397
- Plönjes, E., see Schulz, O. 298 (1998) 385
- Pluta, T. and A.J. Sadlej, HyPol basis sets for high-level-correlated calculations of electric dipole hyperpolarizabilities 297 (1998) 391
- Podgornik, R., see Zihlerl, P. 295 (1998) 99
- Pokrant, S., see Hihara, T. 294 (1998) 357
- Polanyi, J.C., see Zeiri, Y. 300 (1999) 523
- Polavarapu, P.L. and C. Zhao, A comparison of ab initio optical rotations obtained with static and dynamic methods 296 (1998) 105
- Poliakoff, E.D., see Wu, C. 292 (1998) 167
- Polyansky, O.L., see Császár, A.G. 293 (1998) 317
- Polzonetti, G., G. Iucci, M.V. Russo, G. Paolucci, D. Cocco and G. Capellini, Further insight in chromium growth on the surface of an organometallic polymer film 292 (1998) 515
- Popovic, Z.D., see Khan, M.I. 298 (1998) 309
- Popp, J., see Urlaub, E. 298 (1998) 177

- Porteanu, H., see Lifshitz, E. 295 (1998) 249
- Portella-Oberli, M.T., C. Jeannin, B. Soep, G. Zerza and M. Chergui, Femtosecond study of the rise and decay of carbenes in solution 296 (1998) 323
- Potrzebowski, M.J., see Tekely, P. 291 (1998) 471
- Pouilly, B., see Monnerville, M. 294 (1998) 473
- Prater, K., W.L. Freund and R.M. Bowman, Ultrafast investigations of the photophysics of 4-phenylbenzophenone in solution 295 (1998) 82
- Premvardhan, L. and L. Peteanu, Electroabsorption measurements and ab initio calculations of the dipolar properties of 2-(2'-hydroxyphenyl)-benzothiazole and -benzoxazole: two photostabilizers that undergo excited-state proton transfer 296 (1998) 521
- Presilla-Márquez, J.D., J. Harper, J.A. Sheehy, P.G. Carrick and C.W. Larson, Vibrational spectra of cyclic  $C_8$  in solid argon 300 (1999) 719
- Price, S.D., see Newson, K.A. 294 (1998) 223
- Prins, K.O., see de Langen, M. 299 (1999) 195
- Proskuryakov, I.I., I.B. Klenina, I.V. Borovykh, P. Gast and A.J. Hoff, Photoselection effects in laser flash-induced spin-polarised EPR spectra of the radical pair state  $[P^+ Q_A^-]$  in *Rhodobacter sphaeroides* reaction centers 299 (1999) 566
- Proposito, P., see Casalboni, M. 291 (1998) 167
- Provata, A., P. Falaras and A. Xagas, Fractal features of titanium oxide surfaces 297 (1998) 484
- Pryor, B.A., P.M. Palmer, Y. Chen and M.R. Topp, Identification of dual conformers of Coumarin 153 under jet-cooled conditions 299 (1999) 536
- Pszczółkowski, L., see Kisiel, Z. 291 (1998) 190
- Pupyshev, V.I. and A.V. Scherbinin, The Lenz vector in the confined hydrogen atom problem 295 (1998) 217
- Pusel, A., see Wetterauer, U. 300 (1999) 397
- Putter, M., see von Helden, G. 299 (1999) 171
- Puyuelo, M.P., see González, M. 300 (1999) 603
- Pyykkö, P., see Tokman, M. 291 (1998) 414
- Qian, X., see Cao, X. 299 (1999) 322
- Qian, X., see Ramaker, D.E. 299 (1999) 221
- Qiao, C., see Cao, X. 299 (1999) 322
- Qin, L., see He, L. 300 (1999) 504
- Qin, L.-C., Measuring the true helicity of carbon nanotubes 297 (1998) 23
- Qin, Q., see Wang, X. 300 (1999) 739
- Qiu, X., see Zhou, S. 297 (1998) 77
- Quack, M., see Fehrensens, B. 298 (1998) 320
- Quack, M., see Fehrensens, B. 300 (1999) 312
- Quandt, R., see Min, Z. 296 (1998) 372
- Queralt, J.J., see Sambrano, J.R. 294 (1998) 1
- Rabalais, J.W., see van der Heide, P.A.W. 297 (1998) 350
- Rabitz, H., see Dey, B.K. 297 (1998) 247
- Rademacher, P., see Kovačević, B. 293 (1998) 245
- Radhakrishnan, S., see Somani, P. 292 (1998) 218
- Radloff, W., P. Farmanara, V. Stert, E. Schreiber and J.R. Huber, Ultrafast photodissociation dynamics of electronically excited  $CF_2I_2$  molecules 291 (1998) 173
- Rafferty, B.D., see Herbelin, J.M. 299 (1999) 583



- Ramaker, D.E., X. Qian and W.E. O'Grady, 'Atomic' X-ray absorption fine structure: a new tool for examining electronic and ionic polarization effects 299 (1999) 221
- Ramasami, T., see Subramanian, V. 294 (1998) 285
- Ramasami, T., see Subramanian, V. 295 (1998) 312
- Ramírez, P., see Mafé, S. 294 (1998) 406
- Ramírez, R., E. Hernández, J. Schulte and M.C. Böhm, Nuclear quantum effects in the electronic structure of  $C_2H_4$ : a combined Feynman path integral-ab initio approach 291 (1998) 44
- Rao, B.K., see Weber, S.E. 295 (1998) 175
- Rao, C.N.R., see Flahaut, E. 300 (1999) 236
- Rao, C.N.R., see Satishkumar, B.C. 293 (1998) 47
- Rao, C.N.R., see Satishkumar, B.C. 300 (1999) 473
- Rao, D.V.G.L.N., see Venugopal Rao, S. 297 (1998) 491
- Ratcliffe, C.I., see Ba, Y. 299 (1999) 201
- Räther, G., see Mayer, I. 293 (1998) 81
- Ravishankara, A.R., see Brown, S.S. 299 (1999) 277
- Rayez, J.C., see Bonnet, L. 296 (1998) 19
- Re, N., see De Angelis, F. 291 (1998) 57
- Rector, K.D., see Aubuchon, C.M. 299 (1999) 84
- Reddy, B.V., see Weber, S.E. 295 (1998) 175
- Redlich, Ph., see Banhart, F. 292 (1998) 554
- Rega, N., M. Cossi and V. Barone, Towards linear scaling in continuum solvent models. A new iterative procedure for energies and geometry optimizations 293 (1998) 221
- Reid, K.L., Geometrical effects in the spin polarization of molecular photoelectrons 293 (1998) 127
- Reid, S.A., see Tang, Y. 292 (1998) 691
- Reimann, B., see Hobza, P. 299 (1999) 180
- Reinen, D., see Hu, Z. 297 (1998) 321
- Reinhold, E., W. Hogervorst and W. Ubachs, Complete  $g-u$  symmetry breaking in highly excited valence states of the HD molecule 296 (1998) 411
- Reininger, R., see Evans, C.M. 297 (1998) 127
- Reinot, T., J.M. Hayes, G.J. Small and M.C. Zerner, Q-band splitting and relaxation of aluminum phthalocyanine tetrasulfonate 299 (1999) 410
- Remacle, F., C.P. Collier, J.R. Heath and R.D. Levine, The transition from localized to collective electronic states in a silver quantum dots monolayer examined by nonlinear optical response 291 (1998) 453
- Ren, H.-L., Y. Yue, C.-H. Ye, L.-P. Guo and J.-H. Lei, NMR study of crystallization in  $MgO-CaO-SiO_2-P_2O_5$  glass-ceramics 292 (1998) 317
- Rentsch, S., see Paa, W. 292 (1998) 607
- Requena, A., see Zúñiga, J. 298 (1998) 36
- Rettig, W., see Maus, M. 292 (1998) 115
- Reuse, F.A., see Desmarais, N. 294 (1998) 480
- Reynolds, L., see Mente, S. 293 (1998) 515
- Ricca, A., Accurate  $D_0$  value for  $NF^+$  300 (1999) 80
- Ricca, A., Heats of formation for  $NF_n$  ( $n = 1-3$ ) and  $NF_n^+$  ( $n = 1-3$ ) 294 (1998) 454
- Rice, S.A., see Tam, M.C.-M. 294 (1998) 217
- Richter, R.C., see Hynes, A.J. 295 (1998) 25
- Ridley, T., see O'Keeffe, P. 298 (1998) 368
- Rieder, K.-H., see Bartels, L. 291 (1998) 573
- Rieder, K.-H., see Bartels, L. 297 (1998) 287

- Riedle, E., see Wurzer, A.J. 299 (1999) 296
- Riehn, C., A. Weichert, M. Zimmermann and B. Brutschy, Rotational coherence spectroscopy of *para*-difluorobenzene-Ar 299 (1999) 103
- Rienstra-Kiracofe, J.C., see Yamaguchi, Y. 291 (1998) 509
- Rigler, R., see Edman, L. 292 (1998) 15
- Rigler, R., see Edman, L. 294 (1998) 625
- Rinzler, A.G., see Hafner, J.H. 296 (1998) 195
- Rinzler, A.G., see Mickelson, E.T. 296 (1998) 188
- Ríos, M.A., see Cabaleiro-Lago, E.M. 294 (1998) 272
- Ríos, M.A., see Cabaleiro-Lago, E.M. 299 (1999) 358
- Ripmeester, J.A., see Ba, Y. 299 (1999) 201
- Risse, T., see Hill, T. 292 (1998) 524
- Ritchie, G.A.D., see Bakker, B.L.G. 294 (1998) 565
- Ritchie, G.L.D., see Coonan, M.H. 293 (1998) 197
- Ritchie, G.L.D., see Lamb, D.W. 291 (1998) 197
- Rizzo, A., see Coriani, S. 293 (1998) 324
- Rizzo, A., see Coriani, S. 300 (1999) 61
- Robb, M.A., see Klein, S. 292 (1998) 259
- Roberts, J.D., see Zhong, D. 298 (1998) 129
- Robin, P., see Dupuis, B. 300 (1999) 169
- Robinson, J.S., see Allen, M.D. 293 (1998) 397
- Rocheffort, A., D.R. Salahub and P. Avouris, The effect of structural distortions on the electronic structure of carbon nanotubes 297 (1998) 45
- Rodrigues, S.P.J., see Varandas, A.J.C. 297 (1998) 458
- Rodriguez, J.A., S. Chaturvedi and T. Jirsak, The bonding of sulfur to Pd surfaces: photoemission and molecular-orbital studies 296 (1998) 421
- Roeselová, M., G. Jacoby, U. Kaldor and P. Jungwirth, Relaxation of chlorine anions solvated in small water clusters upon electron photodetachment. The three lowest potential energy surfaces of the neutral  $\text{Cl}^- \cdots \text{H}_2\text{O}$  complex 293 (1998) 309
- Rogers, K.M., see Fowler, P.W. 299 (1999) 359
- Rogers, K.M., see Fowler, P.W. 300 (1999) 369
- Roland, C., see Buongiorno Nardelli, M. 296 (1998) 471
- Roman, V.E., see Urlaub, E. 298 (1998) 177
- Romero, T., J. de Andrés, J. Sogas, J.M. Bocanegra, M. Albertí, J.M. Lucas and A. Aguilar,  $\text{Rb}(5^2\text{P}_{1/2,3/2})$  and  $\text{Rb}(6^2\text{P}_{1/2,3/2})$  formation in  $\text{Rb}(5^2\text{S}_{1/2}) + \text{Rb}^+(^1\text{S}_0)$  collisions by crossed molecular beams 292 (1998) 323
- Rommens, J., M. Van der Auweraer and F.C. De Schryver, Sensitized photocurrents in molecular dispersions of 5'-[4-[bis(4-ethylphenyl)amino]phenyl]-N,N,N',N'-tetrakis(4-ethylphenyl)-[1,1':3',1''-terphenyl]-4,4''-diamine 294 (1998) 434
- Roos, B.O., see Serrano-Andrés, L. 295 (1998) 195
- Rösch, N., see Matveev, A.V. 299 (1999) 603
- Rösch, N., see Pacchioni, G. 299 (1999) 137
- Rösch, N., see Voityuk, A.A. 296 (1998) 269
- Rosén, A., see Holmgren, L. 296 (1998) 167
- Rosendahl, A.R., see Hynes, A.J. 295 (1998) 25
- Rössling, G., see Urlaub, E. 298 (1998) 177
- Rost, J.M., see Pattard, T. 291 (1998) 360
- Rosta, E., see Ángyán, J.G. 299 (1999) 1

- Rotermund, H.H., see Kelling, S. 293 (1998) 325
- Roth, D., see Dopfer, O. 296 (1998) 585
- Roth, D.A., M. Hepp, I. Pak and G. Winnewisser, Unequivocal laboratory detection of CO dimer transitions in the millimeter wave region 298 (1998) 381
- Roth, D.A., see Linnartz, H. 292 (1998) 188
- Röthlisberger, U., see Doclo, K. 297 (1998) 205
- Rougeau, N. and C. Kubach, Model quantum study of the  $\text{H}_2\text{O} + \text{Cl} \rightarrow \text{OH} + \text{HCl}$  reaction 299 (1999) 120
- Rousseau, R., G. Dietrich, S. Krückeberg, K. Lützenkirchen, D. Marx, L. Schweikhard and C. Walther, Probing cluster structures with sensor molecules: methanol adsorbed onto gold clusters 295 (1998) 41
- Rousset, A., see Flahaut, E. 300 (1999) 236
- Roux, B., see Chakrabarti, N. 293 (1998) 209
- Rowat, T.E., see Gough, T.E. 298 (1998) 196
- Roy, A.K. and B.M. Deb, Density functional calculations on neon satellites 292 (1998) 461
- Roy, A.K., see Singh, R. 296 (1998) 530
- Rozière, J., see Lamrabte, A. 295 (1998) 257
- Rubahn, H.-G., see Balzer, F. 297 (1998) 273
- Rubin, M.B., see Schael, F. 296 (1998) 592
- Rubio, A., see Gritsenko, O.V. 296 (1998) 307
- Rubio, M., see Serrano-Andrés, L. 295 (1998) 195
- Rubner, O. and V. Engel, Fragmentation dynamics of  $\text{Fe}(\text{CO})_5$  upon femtosecond excitation: a time-dependent statistical description 293 (1998) 485
- Rudert, A.D., J. Martin, H. Zacharias and J.B. Halpern, Controlling molecular angular momentum orientation by Raman pumping and optical ac Stark effect 294 (1998) 381
- Ruggiero, S.T., see Nolen, S. 300 (1999) 656
- Rui, M., see Magnasco, V. 291 (1998) 529
- Ruiz-López, M.F., see Li, G.-S. 297 (1998) 38
- Ruiz-López, M.F., see Salvatella, L. 296 (1998) 239
- Runge, K., B.G. Sumpter, D.W. Noid and M.D. Barnes, Chemical potential and symmetry properties for excess electrons on polymer nanoparticles: quantum drops 299 (1999) 352
- Ruoff, P., A. Bjørnstad and M. Jakobsen, The complete UV–visible photoluminescence spectrum of aqueous  $\text{Ce}(\text{III})$  291 (1998) 249
- Russo, M.V., see Polzonetti, G. 292 (1998) 515
- Russo, N., see Mele, F. 295 (1998) 409
- Rustici, M., M. Branca, A. Brunetti, C. Caravati and N. Marchettini, Inverse Ruelle–Takens–Newhouse scenario in a closed unstirred cerium-catalysed Belousov–Zhabotinsky system 293 (1998) 145
- Rüterjans, H., see Karimi-Nejad, Y. 300 (1999) 706
- Ruth, U., see Jänsch, H.J. 296 (1998) 146
- Ruud, K., J. Vaara, J. Lounila and T. Helgaker, Vibrationally averaged magnetizabilities and rotational  $g$  tensors of the water molecule 297 (1998) 467
- Ruud, K., see Coriani, S. 300 (1999) 61
- Ruud, K., see Minaev, B. 295 (1998) 455
- Sadlej, A.J., see Kellö, V. 292 (1998) 403
- Sadlej, A.J., see Pluta, T. 297 (1998) 391
- Sadr-Lahijany, M.R., see Canpolat, M. 294 (1998) 9
- Saeki, M., see Tsukuda, T. 295 (1998) 416



- Sáez Rábanos, V., see Aoiz, F.J. 299 (1999) 25
- Safi, B., K. Choho, F. De Proft and P. Geerlings, Theoretical study of the basicity of alkyl amines in vacuo and in different solvents: a density functional theory approach 300 (1999) 85
- Safont, V.S., see Oliva, M. 294 (1998) 87
- Sagun, E., see Knyukshto, V. 297 (1998) 97
- Saija, F., see Costa, D. 291 (1998) 252
- Saija, F., see Costa, D. 299 (1999) 252
- Saito, I., see Yoshioka, Y. 294 (1998) 459
- Saito, N., H. Nishiyama, K. Sato and Y. Inoue, Artificial control of selectivity for ethanol decomposition on a Ag catalyst by thickness-extensional mode resonance oscillation of  $z$ -cut  $\text{LiNbO}_3$  297 (1998) 72
- Saito, N., K. Koyama and M. Tanimoto, The stability of multiply charged vanadium, niobium and tantalum clusters 300 (1999) 262
- Saito, Y., Y. Tani, N. Miyagawa, K. Mitsushima, A. Kasuya and Y. Nishina, High yield of single-wall carbon nanotubes by arc discharge using Rh–Pt mixed catalysts 294 (1998) 593
- Saito, Y., see Sugano, M. 292 (1998) 575
- Saitow, K., N. Ichinose, S. Kawanishi and H. Fukumura, Effect of hydrogen bonding on laser-induced transfer of 1-pyrenebutyric acid in solid polymers 291 (1998) 433
- Sakano, M., see Terada, S. 300 (1999) 645
- Sakata, M., see Nishibori, E. 298 (1998) 79
- Sakata, T., see Ohtake, T. 298 (1998) 395
- Sakellariou, D., P. Hodgkinson and L. Emsley, Quasi equilibria in solid-state NMR 293 (1998) 110
- Sako, T., A. Hishikawa and K. Yamanouchi, Vibrational propensity in the predissociation rate of  $\text{SO}_2(\tilde{\text{C}}^1\text{B}_2)$  by two types of nodal patterns in vibrational wavefunctions 294 (1998) 571
- Sako, T., K. Yamanouchi and F. Iachello, Algebraic force-field Hamiltonian expansion for a strongly anharmonic potential: application to the  $\tilde{\text{C}}$  state of  $\text{SO}_2$  299 (1999) 35
- Sakurai, M., see Houjou, H. 294 (1998) 162
- Sakurai, M., see Yamane, T. 291 (1998) 137
- Salahub, D.R., see Rochefort, A. 297 (1998) 45
- Salkola, M.I., Excitons versus continuum states of electrons and holes in solid  $\text{C}_{60}$ : an estimate for the band edge 297 (1998) 499
- Salvatella, L., A. Mokrane, A. Cartier and M.F. Ruiz-López, Combined AM1/MM3 computations on organic systems: the Diels–Alder reaction as a test case 296 (1998) 239
- Salveti, G., see Tombari, E. 300 (1999) 749
- Sambrano, J.R., A.R. de Sousa, J.J. Queralt, J. Andrés and E. Longo, A theoretical analysis on the intramolecular proton transfer of  $\alpha$ -alanine in an aqueous medium 294 (1998) 1
- Sameshima, K., see Houjou, H. 294 (1998) 162
- Samoson, A., see Pingel, U.-T. 294 (1998) 345
- Samuels, D.A. and R.B. Weisman, A new photometric method for directly determining molar absorptivity–quantum yield products of excited states: application to triplet  $\text{C}_{60}$  295 (1998) 105
- Sánchez, F., see García-Ochoa, I. 296 (1998) 335
- Sánchez-Marín, J., see Pérez-Casany, M.P. 295 (1998) 181
- Sánchez-Marín, J., see Pitarch-Ruiz, J. 291 (1998) 407
- Sancho-García, J.C., see Moscardó, F. 294 (1998) 314
- Sandall, J.P.B., see Fowler, P.W. 300 (1999) 369
- Sanders, J.K.M., see Thomas, P.J. 294 (1998) 229
- Sandström, D., M. Hong and K. Schmidt-Rohr, Identification and mobility of deuterated residues in peptides and proteins by  $^2\text{H}$ – $^{13}\text{C}$  solid-state NMR 300 (1999) 213

- Sannigrahi, A.B. and T. Kar, Some remarks on multi-center bond index 299 (1999) 518
- Santos, L., see García-Ochoa, I. 296 (1998) 335
- Sarfatti, J., see Levit, C. 297 (1998) 263
- Sasaki, K., see Yoshikawa, H. 293 (1998) 185
- Sashima, T., H. Nagae, M. Kuki and Y. Koyama, A new singlet-excited state of all-*trans*-spheroidene as detected by resonance-Raman excitation profiles 299 (1999) 187
- Sassara, A., see Brunetti, B. 294 (1998) 584
- Sastre, R., see Arbeloa, T.L. 299 (1999) 315
- Sasuga, T., see Hatanaka, K. 300 (1999) 727
- Satishkumar, B.C., A. Govindaraj, K.R. Harikumar, J.-P. Zhang, A.K. Cheetham and C.N.R. Rao, Boron-carbon nanotubes from the pyrolysis of C<sub>2</sub>H<sub>2</sub>-B<sub>2</sub>H<sub>6</sub> mixtures 300 (1999) 473
- Satishkumar, B.C., A. Govindaraj, R. Sen and C.N.R. Rao, Single-walled nanotubes by the pyrolysis of acetylene-organometallic mixtures 293 (1998) 47
- Sato, K., see Saito, N. 297 (1998) 72
- Sato, T., see Han, W. 299 (1999) 368
- Saue, T., see Ismail, N. 300 (1999) 296
- Sauer, J., see Hübner, O. 294 (1998) 37
- Sauer, S.P.A., A relation between the rotational *g*-factor and the electric dipole moment of a diatomic molecule 297 (1998) 475
- Saunders, V.R., see Civalleri, B. 292 (1998) 394
- Sautet, P., see Loffreda, D. 291 (1998) 15
- Sautet, P., see Pedersen, M.Ø. 299 (1999) 403
- Sauvajol, J.-L., see Lamrabte, A. 295 (1998) 257
- Sauvajol, J.-L., see Maser, W.K. 292 (1998) 587
- Sawa, T., see Sueki, K. 300 (1999) 140
- Sawamura, S. and N. Fujita, Anomalous pressure dependence of the solubility of C<sub>60</sub> in *n*-hexane 299 (1999) 177
- Saykally, R.J., see Cruzan, J.D. 292 (1998) 667
- Saykally, R.J., see Kraus, D. 295 (1998) 285
- Sayós, R., see González, M. 300 (1999) 603
- Scacco, A., see Martini, M. 293 (1998) 43
- Scala, A., see Canpolat, M. 294 (1998) 9
- Scandella, L., see Berger, R. 294 (1998) 363
- Scappini, F., see Tamassia, F. 300 (1999) 478
- Schaafsma, T.J., see Kerp, H.R. 298 (1998) 302
- Schaefer III, H.F., see Yamaguchi, Y. 291 (1998) 509
- Schael, F., M.B. Rubin and S. Speiser, Intramolecular relaxation processes in a singlet excited naphthalene-acridine bichromophoric molecule in solution and in a supersonic jet expansion 296 (1998) 592
- Schäfer, J., J. Wolfrum, R.A. Fischer and H. Sussek, Monitoring of H<sub>y</sub>GaN<sub>x</sub> and Ga in OMCVD of GaN, using molecular beam quadrupole and REMPI-TOF mass spectrometry 300 (1999) 152
- Schäfer, R., see Bachels, T. 300 (1999) 177
- Schatz, G.C., see Ishida, T. 298 (1998) 285
- Scheblykin, I.G., O.P. Varnavsky, M.M. Bataiev, O. Sliusarenko, M. Van der Auweraer and A.G. Vitukhnovsky, Non-coherent exciton migration in J-aggregates of the dye THIATS: exciton-exciton annihilation and fluorescence depolarization 298 (1998) 341

- Schenker, S., A. Hauser, W. Wang and I.Y. Chan, Matrix effects on the high-spin  $\rightarrow$  low-spin relaxation in  $[M_{1-x}Fe_x(bpy)_3](PF_6)_2$  ( $M = Cd, Mn$  and  $Zn$ ,  $bpy = 2,2'$ -bipyridine) 297 (1998) 281
- Scherbinin, A.V., see Pupyshev, V.I. 295 (1998) 217
- Scherer, J.J., Ringdown spectral photography 292 (1998) 143
- Schimmelpfennig, B., see Malkina, O.L. 296 (1998) 93
- Schinke, R., see Hauschildt, J. 300 (1999) 569
- Schipper, D., see Karimi-Nejad, Y. 300 (1999) 706
- Schirrmeister, D.H. and V. May, Femtosecond pulse dependence of dissipation in molecular systems 297 (1998) 383
- Schiwek, M., see Gerhards, M. 297 (1998) 515
- Schlag, E.W., see Baranov, L.Ya. 291 (1998) 311
- Schlag, E.W., see Held, A. 291 (1998) 318
- Schlag, E.W., see Held, A. 299 (1999) 110
- Schmalz, A., see Kanzow, H. 295 (1998) 525
- Schmalz, T.G., see Flocke, N. 298 (1998) 71
- Schmidt, J., see Hill, T. 292 (1998) 524
- Schmidt, J., see Jänsch, H.J. 296 (1998) 146
- Schmidt, J., see van Oijen, A.M. 292 (1998) 183
- Schmidt-Rohr, K., see Sandström, D. 300 (1999) 213
- Schmidt, Th., see Sonnleitner, M. 300 (1999) 221
- Schmidt, T.W., G.B. Bacskey and S.H. Kable, Ab initio potential energy surface and vibrational frequencies of  $\tilde{A}(^1A'')$  HCF 292 (1998) 80
- Schmidtke, H.-H., see Mink, H.J. 291 (1998) 202
- Schneider-Kühnle, Y., T. Dreier and J. Wolfrum, Vibrational relaxation and energy transfer in the hydrogen system at temperatures between 110 and 300 K 294 (1998) 191
- Scholes, G.D., G.O. Turner, K.P. Ghiggino, M.N. Paddon-Row, J.J. Piet, W. Schuddeboom and J.M. Warman, Electronic interactions in rigidly linked naphthalene dimers 292 (1998) 601
- Schreiber, E., see Radloff, W. 291 (1998) 173
- Schroeder, J., see Heidelberg, C. 291 (1998) 333
- Schuddeboom, W., see Scholes, G.D. 292 (1998) 601
- Schulte, J., see Ramírez, R. 291 (1998) 44
- Schulz, K.J. and W.R. Simpson, Frequency-matched cavity ring-down spectroscopy 297 (1998) 523
- Schulz, O., E. Plönjes and W. Urban, Laser action in an optically pumped carbon monoxide plasma 298 (1998) 385
- Schumm, S., see Gerhards, M. 294 (1998) 65
- Schüßler-Langeheine, C., see Meier, R. 292 (1998) 507
- Schütz, G.J., see Sonnleitner, M. 300 (1999) 221
- Schwartz, R.L., see Krause, P.J. 294 (1998) 518
- Schwarzer, D., see Heidelberg, C. 291 (1998) 333
- Schweig, A., see Zimmer, K. 293 (1998) 366
- Schweigert, V., see Meleshko, V. 300 (1999) 118
- Schweikhard, L., see Rousseau, R. 295 (1998) 41
- Schweitzer, G., see Latterini, L. 295 (1998) 11
- Schwerdtfeger, P., see Pernpointner, M. 295 (1998) 347
- Scott, J.C. and G.G. Malliaras, Charge injection and recombination at the metal-organic interface 299 (1999) 115
- Scovell, D.L., T.D. Pinkerton, B.A. Finlayson and E.M. Stuve, The dielectric response of water in high electric fields: equilibrium water thickness and the field distribution 294 (1998) 255



- Scuseria, G.E., see Boese, A.D. 294 (1998) 233
- Seccombe, D.P., see Boyle, K.J. 294 (1998) 507
- Seifert, G., see Fowler, P.W. 299 (1999) 359
- Seifert, G., see Fowler, P.W. 300 (1999) 369
- Seijo, L., see Díaz-Megías, S. 299 (1999) 613
- Seimiya, Y., see Cao, G. 294 (1998) 419
- Seki, K., see Noda, M. 296 (1998) 599
- Sekine, T., see Awaga, K. 293 (1998) 352
- Sekkat, Z., see Ishitobi, H. 300 (1999) 421
- Seko, T., K. Ogura, Y. Kawakami, H. Sugino, H. Toyotama and J. Tanaka, Excimer emission of anthracene, perylene, coronene and pyrene microcrystals dispersed in water 291 (1998) 438
- Selloni, A., see De Angelis, F. 291 (1998) 57
- Selzle, H.L., see Baranov, L.Ya. 291 (1998) 311
- Selzle, H.L., see Held, A. 291 (1998) 318
- Selzle, H.L., see Held, A. 299 (1999) 110
- Semenov, S.K. and N.A. Cherepkov, Generalization of the atomic RPA method for diatomic molecules: H<sub>2</sub> photoionization cross-section calculation 291 (1998) 375
- Semkin, V.N., N.V. Drichko, Yu.A. Kumzerov, D.V. Konarev, R.N. Lyubovskaya and A. Graja, The orientational-ordering transition in single crystals of selected C<sub>60</sub> complexes with organic donors followed by infrared spectroscopy 295 (1998) 266
- Sen, A. and V. Krishnan, Novel covalently linked porphyrin dimers for controlled intramolecular energy transfer 294 (1998) 499
- Sen, R., see Satishkumar, B.C. 293 (1998) 47
- Senent, M.L., Determination of the kinetic energy parameters of non-rigid molecules 296 (1998) 299
- Senesi, R., see Casalboni, M. 291 (1998) 167
- Senet, P., J.P. Toennies and G. Witte, Low-frequency vibrations of alkali atoms on Cu(001) 299 (1999) 389
- Sengupta, P.K., see Falkovskaia, E. 297 (1998) 109
- Senn, G., see Brüning, F. 292 (1998) 177
- Sepiół, J., Y. Stepanenko, A. Vdovin, A. Mordziński, E. Vogel and J. Waluk, Proton tunnelling in porphycene seeded in a supersonic jet 296 (1998) 549
- Sepiół, J., see Vdovin, A. 296 (1998) 557
- Serrano-Andrés, L., M. Merchán, M. Rubio and B.O. Roos, Interpretation of the electronic absorption spectrum of free base porphyrin by using multiconfigurational second-order perturbation theory 295 (1998) 195
- Sessler, J.L., see Shuali, Z. 300 (1999) 687
- Seta, P., see Lamrabte, A. 295 (1998) 257
- Setser, D.W., see Hewett, K.B. 297 (1998) 335
- Seyller, Th., M. Caragiu, R.D. Diehl, P. Kaukasoina and M. Lindroos, Observation of top-site adsorption for Xe on Cu(111) 291 (1998) 567
- Seynaeve, E., see Ahlskog, M. 300 (1999) 202
- Sgamellotti, A., see De Angelis, F. 291 (1998) 57
- Shaik, S., see Wu, W. 292 (1998) 7
- Shalagin, A.M., see Il'ichov, L.V. 297 (1998) 439
- Shalashilin, D.V. and B. Jackson, Initial value representation for the classical propagator and S-matrix with the help of coherent states 291 (1998) 143
- Shang, R.C., see Pang, W.N. 296 (1998) 605
- Shang, R.C., see Pang, W.N. 299 (1999) 207
- Sharma, R.K., W.A. Brown and D.A. King, Adsorbed CO chain condensation and evaporation on Pt(110)-(1 × 2) at 30-70 K studied by RAIRS 291 (1998) 1

- Sharma, R.K., see Brown, W.A. 299 (1999) 253
- Sharonov, A., see Lampre, I. 293 (1998) 423
- Sheehy, J.A., see Presilla-Márquez, J.D. 300 (1999) 719
- Shehadi, I.A., L.F. Murga, M.J. Ondrechen and J. Linderberg, A Hubbard model for the second hyperpolarizability in alternating polymers 291 (1998) 325
- Shen, X., M. Belletête and G. Durocher, Study of the interactions between substituted 2,2'-bithiophenes and cyclodextrins 298 (1998) 201
- Shen, Z.X., see He, L. 300 (1999) 504
- Shepard, R., see Müller, T. 293 (1998) 72
- Shiga, M. and S. Okazaki, A molecular dynamics study of the vibrational energy relaxation of the cyanide ion in aqueous solution 292 (1998) 431
- Shigemasa, E., see Adachi, J. 294 (1998) 559
- Shimada, T., H. Taira and A. Koma, Epitaxial growth of squaric acid 291 (1998) 419
- Shimobe, Y., see Jamali, J.B. 292 (1998) 661
- Shin, K.J., see Kim, H. 291 (1998) 341
- Shin, S., see Kim, H. 291 (1998) 341
- Shinohara, H., see Hino, S. 300 (1999) 145
- Shinohara, H., see Nishibori, E. 298 (1998) 79
- Shinohara, H., see Wang, C.-R. 300 (1999) 379
- Shiotani, M., see Komaguchi, K. 300 (1999) 257
- Shiotani, M., see Wang, P. 292 (1998) 110
- Shiraishi, Y., see Sugita, A. 296 (1998) 365
- Shoute, L.C.T., see Pan, D. 292 (1998) 677
- Shuali, Z., A. Berg, H. Levanon, E. Vogel, M. Bröring, J.L. Sessler, C. Fowler and S.J. Weghorn, Photoexcited triplet-state dynamics of novel porphyrinoids: octaethylcorphycene and octaethylhemiporphycene. Time-resolved electron paramagnetic resonance study 300 (1999) 687
- Shukla, A., M. Dolg and H. Stoll, A Wannier-function-based ab initio Hartree–Fock study of polyethylene 294 (1998) 126
- Shulga, A., see Knyukshto, V. 297 (1998) 97
- Shultz, M.J., see Simonelli, D. 298 (1998) 400
- Sidis, V., see Jeloica, L. 300 (1999) 157
- Siebbeles, L.D.A., see Berlin, Y.A. 291 (1998) 85
- Siegbahn, P.E.M., M.R.A. Blomberg and M. Pavlov, A comparison of electron transfer in ribonucleotide reductase and the bacterial photosynthetic reaction center 292 (1998) 421
- Siegel, J.S., see Grunnet-Jepsen, A. 291 (1998) 553
- Siglow, K., R. Neuhauser and H.J. Neusser, Rotational analysis of the ground state of the Benzene · Ne van der Waals cluster cation by resolved high Rydberg spectroscopy 293 (1998) 19
- Silbey, R.J., see Brown, F.L.H. 292 (1998) 357
- Silbey, R.J., see den Hartog, F.T.H. 297 (1998) 314
- Silvi, B., see Krokidis, X. 292 (1998) 35
- Simeonidis, K., see Laenen, R. 292 (1998) 631
- Simeonidis, K., see Laenen, R. 299 (1999) 589
- Simon, D., see Loffreda, D. 291 (1998) 15
- Simon, M., F. Träger, A. Assion, B. Lang, S. Voll and G. Gerber, Femtosecond time-resolved second-harmonic generation at the surface of alkali metal clusters 296 (1998) 579
- Simonelli, D., S. Baldelli and M.J. Shultz, Ammonia–water complexes on the surface of aqueous solutions observed with sum frequency generation 298 (1998) 400

- Simonson, J.M., see Lee, S.H. 293 (1998) 289
- Simper, A.M., see Skylaris, C.-K. 296 (1998) 445
- Simpson, W.R., see Schulz, K.J. 297 (1998) 523
- Singh, R., A.K. Roy and B.M. Deb, Density functional calculations on low-lying singly excited states of open-shell atoms 296 (1998) 530
- Singh, R.K., P. Bhargavansh, B.P. Asthana and A.L. Verma, Raman study of vibrational dephasing in hydrogen-bonded binary and ternary complexes of  $C_6H_5Cl$  and methanol 296 (1998) 611
- Singhal, R.P., H.S. Kilic, K.W.D. Ledingham, T. McCanny, W.X. Peng, D.J. Smith, C. Kosmidis, A.J. Langley and P.F. Taday, Comment on "On the ionisation and dissociation of  $NO_2$  by short intense laser pulses" 292 (1998) 643
- Sinnott, S.B., see Garg, A. 295 (1998) 273
- Sivanesan, D., see Subramanian, V. 294 (1998) 285
- Sivanesan, D., see Subramanian, V. 295 (1998) 312
- Skaf, M.S., see Borin, I.A. 296 (1998) 125
- Skinner, D.E. and W.H. Miller, Application of the semiclassical initial value representation and its linearized approximation to inelastic scattering 300 (1999) 20
- Skinner, J.L., see Egorov, S.A. 293 (1998) 469
- Skipper, N.T., see Walters, J.K. 300 (1999) 444
- Skurski, P., see Gutowski, M. 300 (1999) 331
- Skylaris, C.-K., L. Gagliardi, N.C. Handy, A.G. Ioannou, S. Spencer, A. Willetts and A.M. Simper, An efficient method for calculating effective core potential integrals which involve projection operators 296 (1998) 445
- Slaviček, P., D. Nachtigallova and P. Jungwirth, First electronically excited state of the water-argon complex: an analytical fit to the CASPT2 potential 300 (1999) 561
- Sliusarenko, O., see Scheblykin, I.G. 298 (1998) 341
- Sluyts, E.J., see Herrebout, W.A. 295 (1998) 223
- Small, G.J., see Reinot, T. 299 (1999) 410
- Smalley, R.E., see Hafner, J.H. 296 (1998) 195
- Smalley, R.E., see Mickelson, E.T. 296 (1998) 188
- Smets, J., D.M.A. Smith and L. Adamowicz, Ab initio theoretical study of dipole-bound anions of molecular complexes. Anions of H-bonded hydrogen cyanide polymers 297 (1998) 451
- Smith, B., see Grunnet-Jepsen, A. 291 (1998) 553
- Smith, B.R., see Klein, S. 292 (1998) 259
- Smith, D.J., see Singhal, R.P. 292 (1998) 643
- Smith, D.M.A., see Smets, J. 297 (1998) 451
- Smith, I.W.M., see Henton, S. 291 (1998) 223
- Smith, K.A., see Hafner, J.H. 296 (1998) 195
- Smith, M.A., see Ahern, M.M. 300 (1999) 681
- Smith, M.L., see Edholm, O. 291 (1998) 501
- Snijders, J.G., see de Lange, M.J.L. 294 (1998) 332
- So, S.P., Theoretical study of  $Ge_5H_5^+$  isomers 291 (1998) 523
- Sobolewski, A.L. and W. Domcke, On the mechanism of rapid non-radiative decay in intramolecularly hydrogen-bonded  $\pi$  systems 300 (1999) 533
- Soejima, Y., see Jamali, J.B. 292 (1998) 661
- Soep, B., see Portella-Oberli, M.T. 296 (1998) 323
- Sogas, J., see Romero, T. 292 (1998) 323
- Soldán, P., see Lee, E.P.F. 295 (1998) 354
- Soldatović, T., see Gutman, I. 297 (1998) 428



- Somani, P. and S. Radhakrishnan, Electrochromic response in polypyrrole sensitized by Prussian blue 292 (1998) 218
- Someda, K., see Hashimoto, N. 291 (1998) 130
- Sonnleitner, M., G.J. Schütz and Th. Schmidt, Imaging individual molecules by two-photon excitation 300 (1999) 221
- Sonoyama, N., see Ohtake, T. 298 (1998) 395
- Soper, A.K., see Walters, J.K. 300 (1999) 444
- Soudackov, A.V. and S. Hammes-Schiffer, Removal of the double adiabatic approximation for proton-coupled electron transfer reactions in solution 299 (1999) 503
- Sousa, L.R., see Bhattacharyya, S. 297 (1998) 154
- Space, B., see Moore, P.B. 296 (1998) 259
- Spanget-Larsen, J., see Møller, S. 291 (1998) 51
- Speiser, S., see Schael, F. 296 (1998) 592
- Spencer, S., see Skylaris, C.-K. 296 (1998) 445
- Spiegelmann, F., see Zhang, F.S. 300 (1999) 595
- Spiering, H., see Ksenofontov, V. 294 (1998) 545
- Spiess, H.W., see Jeschke, G. 293 (1998) 9
- Špirko, V., see Hobza, P. 299 (1999) 180
- Spoerel, U., see Consalvo, D. 297 (1998) 543
- Springborg, M., see Meider, H. 300 (1999) 339
- Srivastava, A. and K.B. Eisenthal, Kinetics of molecular transport across a liposome bilayer 292 (1998) 345
- Stace, A.J., see Walker, N.R. 292 (1998) 125
- Staemmler, V., see Klüner, T. 294 (1998) 413
- Stahl, D., see Jänsch, H.J. 296 (1998) 146
- Stanley, H.E., see Canpolat, M. 294 (1998) 9
- Stanton, J.F., see Christiansen, O. 292 (1998) 437
- Stanton, J.F., see Gauss, J. 296 (1998) 117
- Starikovskaia, S.M., see Pancheshnyi, S.V. 294 (1998) 523
- Starikovskii, A.Y., see Pancheshnyi, S.V. 294 (1998) 523
- Staroverov, V.N. and E.R. Davidson, The reduced model space method in multireference second-order perturbation theory 296 (1998) 435
- Starr, F.W., see Canpolat, M. 294 (1998) 9
- Staško, A., see Brezová, V. 300 (1999) 667
- Stass, D.V., see Sviridenko, F.B. 297 (1998) 343
- Stefanovich, E.V. and T.N. Truong, Ab initio study of water adsorption on  $\text{TiO}_2(110)$ : molecular adsorption versus dissociative chemisorption 299 (1999) 623
- Steiger, B., see Yu, H.Z. 293 (1998) 1
- Steinhurst, D.A., see Ahern, M.M. 300 (1999) 681
- Stelzer, J., R. Berardi and C. Zannoni, Flexoelectric effects in liquid crystals formed by pear-shaped molecules. A computer simulation study 299 (1999) 9
- Stempel, S., see Hill, T. 292 (1998) 524
- Stensgaard, I., see Pedersen, M.Ø. 299 (1999) 403
- Stepanenko, Y., see Sepiół, J. 296 (1998) 549
- Stepanian, S., see Alexandrov, V. 291 (1998) 110
- Stephens, J.C., see Yamaguchi, Y. 291 (1998) 509
- Stert, V., see Radloff, W. 291 (1998) 173
- Stevens, M.G., S. Subramoney and H.C. Foley, Spontaneous formation of carbon nanotubes and polyhedra from cesium and amorphous carbon 292 (1998) 352

- Stimson, M.J., see Kirkwood, J.C. 293 (1998) 417
- Stirling, A., Theoretical calculations on the reactions of NO<sub>2</sub> with Sc, Ti and V 298 (1998) 101
- Stock, G., see Hahn, S. 296 (1998) 137
- Stoeckel, F., see Garnache, A. 292 (1998) 698
- Stoll, H., see Fulde, P. 299 (1999) 481
- Stoll, H., see Shukla, A. 294 (1998) 126
- Stolov, A.A., see Herrebout, W.A. 295 (1998) 223
- Stolte, S., see de Lange, M.J.L. 294 (1998) 332
- Straková, P., see Nikl, M. 291 (1998) 300
- Strasser, J., H. Yersin and H.H. Patterson, Effect of high pressure on the emission spectrum of single crystals of Ti[Au(CN)<sub>2</sub>] 295 (1998) 95
- Stratmann, R.E., see Wiberg, K.B. 297 (1998) 60
- Stratt, R.M., see Larsen, R.E. 297 (1998) 211
- Stręk, W., see Dereń, P.J. 298 (1998) 217
- Strzalka, K., see Konopasek, I. 293 (1998) 429
- Stuve, E.M., see Scovell, D.L. 294 (1998) 255
- Su, M.-D. and S.-Y. Chu, Structures and relative stabilities of the novel sandwich complexes related to pentalene: a density functional study 298 (1998) 107
- Suarez, C.B., see Krämer, H.-G. 299 (1999) 212
- Subramanian, V., D. Sivanesan and T. Ramasami, Electronic structure of Ne–H–Cl and Ne–Cl–H using the G1, G2 and MP4 methods 295 (1998) 312
- Subramanian, V., D. Sivanesan, R. Amutha, J. Padmanabhan and T. Ramasami, Hardness profile of interaction of H–F with He, Ne and Ar: a density functional and MP2 calculation 294 (1998) 285
- Subramoney, S., see Stevens, M.G. 292 (1998) 352
- Suda, A., see Umemoto, H. 296 (1998) 203
- Sueki, K., K. Akiyama, K. Kikuchi and H. Nakahara, Specificity of carbon cages towards oxidation states of metal atoms in metallofullerenes 291 (1998) 37
- Sueki, K., K. Kikuchi, K. Akiyama, T. Sawa, M. Katada, S. Ambe, F. Ambe and H. Nakahara, Formation of metallofullerenes with higher group elements 300 (1999) 140
- Suenaga, K., M.P. Johansson, N. Hellgren, E. Broitman, L.R. Wallenberg, C. Colliex, J.-E. Sundgren and L. Hultman, Carbon nitride nanotubulite – densely-packed and well-aligned tubular nanostructures 300 (1999) 695
- Suffritti, G.B., see Fritzsche, S. 296 (1998) 253
- Sugano, M., A. Kasuya, K. Tohji, Y. Saito and Y. Nishina, Resonance Raman scattering and diameter-dependent electronic states in single-wall carbon nanotubes 292 (1998) 575
- Sugawara, K., see Vakhtin, A.B. 299 (1999) 553
- Sugawara, M., Adaptive basis set for quantum mechanical calculation based on hierarchical finite element method 295 (1998) 423
- Sugino, H., see Seko, T. 291 (1998) 438
- Sugita, A., Y. Shiraishi and T. Kobayashi, Femtosecond–picosecond dynamics of the lowest excited singlet state in  $\alpha$ -quinquethiophene 296 (1998) 365
- Sugiyama, T., see Hiraoka, K. 299 (1999) 545
- Suhai, S., see Mayer, I. 293 (1998) 81
- Suhai, S., see Tajkhorshid, E. 299 (1999) 457
- Sukhov, F.F., see Feldman, V.I. 300 (1999) 713
- Sullivan, R.H., see Jabalameli, A. 295 (1998) 135
- Sumi, H., see Asano, T. 294 (1998) 493

- Sumpter, B.G., see Runge, K. 299 (1999) 352  
Sun, C.-C., see Yu, Y.-X. 296 (1998) 131  
Sun, L.F., see Pan, Z.W. 299 (1999) 97  
Sundgren, J.-E., see Suenaga, K. 300 (1999) 695  
Sundholm, D., see Tokman, M. 291 (1998) 414  
Suo, Z., see Wei, X. 300 (1999) 385  
Suraud, E., see Zhang, F.S. 300 (1999) 595  
Surján, P.R., see Ángyán, J.G. 299 (1999) 1  
Suryaprakash, N., see Khetrapal, C.L. 296 (1998) 537  
Sussek, H., see Schäfer, J. 300 (1999) 152  
Suzuki, S., see Ishihara, S. 295 (1998) 475  
Suzuki, T., see Omori, T. 293 (1998) 436  
Suzuki, T., see Tanaka, H. 293 (1998) 541  
Sviridenko, F.B., D.V. Stass and Yu.N. Molin, Estimation of lifetimes of solvent radical cations in liquid alkanes using the level crossing spectroscopy technique 297 (1998) 343  
Svobodova, J., see Konopasek, I. 293 (1998) 429  
Svrček, M., P. Baňacký, S. Biskupič, J. Noga, P. Pelikán and A. Zajac, Adiabatic correction to the energy of molecular systems: the CPHF equivalent of the Born-Handy formula 299 (1999) 151  
Sworakowski, J. and S. Nešpůrek, A straightforward method of analysis of first-order processes with distributed parameters 298 (1998) 21  
Szalay, P.G., see Cremer, D. 292 (1998) 97  
Szichman, H., see Varandas, A.J.C. 295 (1998) 113  
  
Tachikawa, H., A direct molecular orbital dynamics study on the hydrogen atom trapped in crystalline silicon 300 (1999) 577  
Tachiya, M., see Hilczer, M. 295 (1998) 337  
Taday, P.F., see Singhal, R.P. 292 (1998) 643  
Taira, H., see Shimada, T. 291 (1998) 419  
Tajkhorshid, E. and S. Suhai, Dielectric effects due to the environment on the structure and proton affinity of retinal Schiff base models 299 (1999) 457  
Takabayashi, Y., see Kubozono, Y. 298 (1998) 335  
Takada, T., H. Koizumi and T. Ichikawa, Intramolecular hydrogen transfer of excited alkyl radicals in the solid phase 300 (1999) 253  
Takahashi, H., T. Wakabayashi and T. Nitta, A wavepacket analysis of the statistical behaviour of molecules that penetrate a slit-shaped micropore 294 (1998) 95  
Takahashi, Y., Structural model of toluene-solvated C<sub>70</sub> from high-resolution transmission electron microscopy 292 (1998) 547  
Takami, A., see Koga, K. 293 (1998) 180  
Takami, M., see Geng, J. 291 (1998) 277  
Takanashi, H., see Ohkata, Y. 295 (1998) 17  
Takata, M., see Nishibori, E. 298 (1998) 79  
Takata, Y., see Adachi, J. 294 (1998) 559  
Takayanagi, M., see Kudoh, S. 296 (1998) 329  
Takayanagi, T., see Komaguchi, K. 300 (1999) 257  
Takayanagi, T., see Kurosaki, Y. 293 (1998) 59  
Takayanagi, T., see Kurosaki, Y. 299 (1999) 57  
Takeda, K., see Nakatsuji, S. 296 (1998) 159



- Takeda, S., see Morioka, Y. 292 (1998) 625
- Takeo, H., see Kodaira, T. 300 (1999) 499
- Talukdar, R.K., see Brown, S.S. 299 (1999) 277
- Tam, M.C.-M., S.A. Rice and A.H. Marcus, Unusual structure in a quasi-two-dimensional binary colloid fluid 294 (1998) 217
- Tamassia, F., R. Danieli and F. Scappini, Collision-induced radio-frequency transitions in  $\text{CH}_3\text{I}$  300 (1999) 478
- Tamassia, F., see Bizzocchi, L. 293 (1998) 441
- Tameev, A.R., A.A. Kozlov and A.V. Vannikov, Influence of transport site alignment on electron and hole mobilities in polymer films 294 (1998) 605
- Tamsen, F., see Edman, L. 292 (1998) 15
- Tamsen, F., see Edman, L. 294 (1998) 625
- Tan, H., M. Liao, D. Dai and K. Balasubramanian, Potential energy surfaces of NbCO 297 (1998) 173
- Tanaka, H., T. Iiyama, N. Uekawa, T. Suzuki, A. Matsumoto, M. Grün, K.K. Unger and K. Kaneko, Molecular mechanism of capillary condensation of acetonitrile vapor on MCM-41 with the aid of a time-correlation function analysis of IR spectroscopy 293 (1998) 541
- Tanaka, J., see Seko, T. 291 (1998) 438
- Tanaka, K.-i., see Moriwaki, K. 292 (1998) 500
- Tanaka, S., see Nagasono, M. 298 (1998) 141
- Tanaka, T., see Ohtsuki, T. 300 (1999) 661
- Taneda, K. and K. Mori, Full-variational treatment of GTF basis sets for molecular orbitals: application to interactions in the helium dimer under an electrostatic field 298 (1998) 293
- Tang, K.T., see Johann, C. 295 (1998) 158
- Tang, K.T., see Patil, S.H. 295 (1998) 152
- Tang, S.H., see He, L. 300 (1999) 504
- Tang, Y. and S.A. Reid, Multiplex spectroscopy of jet-cooled  $\text{NO}_2$  292 (1998) 691
- Tang, Y.H., see Wang, N. 299 (1999) 237
- Tani, Y., see Saito, Y. 294 (1998) 593
- Taniguchi, Y., see Kato, M. 294 (1998) 626
- Tanimoto, M., see Saito, N. 300 (1999) 262
- Tanimura, Y., see Imamura, Y. 298 (1998) 15
- Tanimura, Y., see Maruyama, Y. 292 (1998) 28
- Tanimura, Y., see Okumura, K. 295 (1998) 298
- Tanner, D.B., see Kamarás, K. 295 (1998) 279
- Tansho, M., see Nishino, Y. 296 (1998) 408
- Tantirungrotechai, Y., see Cohen, A.J. 299 (1999) 465
- Tapia, O., see Oliva, M. 294 (1998) 87
- Tassotto, M., see Gannon, T.J. 300 (1999) 163
- Tate, R.F., see Herbelin, J.M. 299 (1999) 583
- Tatewaki, H., On the location of  $p_\pi$  holes in a high- $T_c$   $\text{YBa}_2\text{Cu}_3\text{O}_7$  superconductor 295 (1998) 399
- Taylor, R., A. Pénicaud and N.J. Tower, Matrix isolation of fullerene-derived  $\text{CO}_2$  at ambient temperature 295 (1998) 481
- Taylor, R., see Barrow, M.P. 293 (1998) 302
- Taylor, T.R., K.R. Asmis, C. Xu and D.M. Neumark, Evolution of electronic structure as a function of size in gallium phosphide semiconductor clusters 297 (1998) 133
- Taylor, T.R., see Asmis, K.R. 295 (1998) 75
- Tekely, P., M.J. Potrzebowski, Y. Dusaosoy and Z. Luz, Measurement of spin diffusion and intermolecular distances between chemically equivalent nuclei in rotating solids 291 (1998) 471

- Telka, M.A., see Cukrowski, A.S. 297 (1998) 402
- Ten-no, S., see Imamura, Y. 298 (1998) 15
- Tennyson, J., see Császár, A.G. 293 (1998) 317
- Terada, S., T. Yokoyama, M. Sakano, M. Kiguchi, Y. Kitajima and T. Ohta, Asymmetric surface structure of SO<sub>2</sub> on Pd(111) studied by total-reflection X-ray absorption fine structure spectroscopy 300 (1999) 645
- Termath, V., see Hübner, O. 294 (1998) 37
- Terrones, H., see Fowler, P.W. 299 (1999) 359
- Terrones, M., see Fowler, P.W. 299 (1999) 359
- Therssen, E., see Mercier, X. 299 (1999) 75
- Thiel, E., see Menzel, R. 291 (1998) 237
- Thiel, S., see Klüner, T. 294 (1998) 413
- Thiel, W., see Filatov, M. 295 (1998) 467
- Thoman Jr., J.W., see Francisco, J.S. 300 (1999) 553
- Thomas, P.J., N. Berovic, P. Laitenberger, R.E. Palmer, N. Bampos and J.K.M. Sanders, Room temperature manipulation of self-organised supramolecular nanostructures with a scanning tunnelling microscope 294 (1998) 229
- Thompson, K., see Makri, N. 291 (1998) 101
- Thomsen, C., see Kuhlmann, U. 294 (1998) 237
- Till, U., C.R. Timmel, B. Brocklehurst and P.J. Hore, The influence of very small magnetic fields on radical recombination reactions in the limit of slow recombination 298 (1998) 7
- Tillett, M.L., see Norwood, T.J. 300 (1999) 429
- Tilocca, A., see Fritzsche, S. 296 (1998) 253
- Timmel, C.R., see Till, U. 298 (1998) 7
- Tobitani, T., see Yanagi, H. 292 (1998) 332
- Todd, M.W., see Krause, P.J. 294 (1998) 518
- Toennies, J.P., see Johann, C. 295 (1998) 158
- Toennies, J.P., see Senet, P. 299 (1999) 389
- Tohji, K., see Sugano, M. 292 (1998) 575
- Tokman, M., D. Sundholm and P. Pyykkö, Nuclear quadrupole moments of gallium isotopes obtained from finite-element MCHF calculations on the  $4p^2P_{3/2}$  state of Ga 291 (1998) 414
- Tokumura, K., K. Nagaosa, Y. Ohta and R. Matsushima, Temperature-dependent tautomer fluorescence spectra of 3',4'-benzo-2'-hydroxychalcone: direct evidence for photoenolization followed by  $Z \rightarrow E$  isomerization in the singlet manifold 295 (1998) 516
- Tolokh, I.S., see Petrov, E.G. 294 (1998) 19
- Tomás, F., see Anane, H. 296 (1998) 277
- Tombari, E., C. Ferrari and G. Salvetti, Heat capacity anomaly in a large sample of supercooled water 300 (1999) 749
- Tomikawa, K., see Kanno, H. 293 (1998) 412
- Tominaga, Y., see Wang, Y. 299 (1999) 576
- Tomizawa, H., see Morioka, Y. 292 (1998) 625
- Tong, X.-M., see Chu, S.-I. 294 (1998) 31
- Topaler, M.S., see Zeiri, Y. 300 (1999) 523
- Topp, M.R., see Palmer, P.M. 292 (1998) 307
- Topp, M.R., see Pryor, B.A. 299 (1999) 536
- Tóthová, M., A. Nagy and Ľ. Treindl, Oscillations in the reduction of permanganate by hydrogen peroxide or by ninhydrin in a batch reactor and mixed-mode oscillations in a continuous-flow stirred tank reactor 299 (1999) 243

- Tower, N.J., see Barrow, M.P. 293 (1998) 302
- Tower, N.J., see Taylor, R. 295 (1998) 481
- Toyoda, S. and M. Fujiki, Photoluminescence and absorption spectra of poly(pentylphenylsilylene). Absence of broad photoluminescence of poly(alkylarylsilylene) around 2.7 eV 293 (1998) 38
- Toyotama, H., see Seko, T. 291 (1998) 438
- Träger, F., see Simon, M. 296 (1998) 579
- Treindl, Ľ., see Tóthová, M. 299 (1999) 243
- Tretiak, S., V. Chernyak and S. Mukamel, Real-space analysis of electronic excitations in free-base ( $H_2P$ ) and magnesium (MgP) porphins 297 (1998) 357
- Trifunac, A.D., see Chemerisov, S.D. 291 (1998) 262
- Tronc, M., see Le Coat, Y. 296 (1998) 208
- Trontelj, Z., see Mrzel, A. 298 (1998) 329
- Trout, N.A., see Alexander, U.N. 299 (1999) 291
- Troya, D., see González, M. 300 (1999) 603
- Truhlar, D.G., Basis-set extrapolation 294 (1998) 45
- Truhlar, D.G., see Zeiri, Y. 300 (1999) 523
- Truong, T.N., see Stefanovich, E.V. 299 (1999) 623
- Tryk, D.A., see Nakabayashi, S. 300 (1999) 409
- Tsai, C.-S., C.-E. Lin, J.-C. Lin and J.-K. Wang, Vibrational dephasing dynamics of the hydrogenated Si(100)- $2 \times 1$  surface revisited: multi-mode dephasing model 295 (1998) 509
- Tsang, S.C., see Harris, P.J.F. 293 (1998) 53
- Tsivgoulis, G.M., see Owrutsky, J.C. 293 (1998) 555
- Tsuchimoto, M. and N. Yoshioka, Magnetic properties of polynuclear oxovanadium(IV) complexes with tetradentate Schiff base ligands 297 (1998) 115
- Tsuchiya, J., see Okutsu, T. 299 (1999) 597
- Tsukiyama, K., see Ogi, Y. 296 (1998) 384
- Tsukuda, T., M. Saeki, L. Zhu and T. Nagata, Formation of  $N_3O_3^-$  anion in  $(NO)_n^-$ : photoelectron spectroscopy and ab initio calculations 295 (1998) 416
- Tsuno, T., see Ohkata, Y. 295 (1998) 17
- Tsutsui, T., see Era, M. 296 (1998) 417
- Tuckett, R.P., see Boyle, K.J. 294 (1998) 507
- Tuckett, R.P., see Jarvis, G.K. 295 (1998) 145
- Tuckey, P.A., see Dubernet, M.-L. 300 (1999) 275
- Tufeu, R., see Monticone, S. 295 (1998) 237
- Turner, D.E., see Pan, B.C. 292 (1998) 75
- Turner, G.O., see Scholes, G.D. 292 (1998) 601
- Twist, C., see Haouz, A. 294 (1998) 197
- Tyliszczak, T., see Eustatiu, I.G. 300 (1999) 676
- Tyliszczak, T., see Neville, J.J. 300 (1999) 451
- Tyndall, G.S., see Phillips, J.A. 296 (1998) 377
- Ubachs, W., see Reinhold, E. 296 (1998) 411
- Uekawa, N., see Tanaka, H. 293 (1998) 541
- Ugliengo, P., see Civalleri, B. 292 (1998) 394
- Ugliengo, P., see Civalleri, B. 294 (1998) 103
- Ugliengo, P., see Civalleri, B. 299 (1999) 443
- Ulness, D.J., see Kirkwood, J.C. 293 (1998) 167



- Ulness, D.J., see Kirkwood, J.C. 293 (1998) 417  
 Umapathy, S., see Biswas, N. 294 (1998) 181  
 Umek, P., see Mrzel, A. 298 (1998) 329  
 Umemoto, H., Leaving-atom isotope effect in the reactions of  $N(2^2D)$  with isotopic hydrogens 292 (1998) 594  
 Umemoto, H., N. Hachiya, E. Matsunaga, A. Suda and M. Kawasaki, Rate constants for the deactivation of  $N(2^2D)$  by simple hydride and deuteride molecules 296 (1998) 203  
 Umishita, K., see Hino, S. 300 (1999) 145  
 Umitani, S., see Gao, X.-C. 297 (1998) 530  
 Unger, K.K., see Tanaka, H. 293 (1998) 541  
 Unterberg, C., see Gerhards, M. 294 (1998) 65  
 Unterberg, C., see Gerhards, M. 297 (1998) 515  
 Urakawa, T., see Kubozono, Y. 298 (1998) 335  
 Urban, W., see Schulz, O. 298 (1998) 385  
 Urisu, T., see Nagasono, M. 298 (1998) 141  
 Urlaub, E., J. Popp, V.E. Roman, W. Kiefer, M. Lankers and G. Rössling, Raman spectroscopic monitoring of the polymerization of cyanacrylate 298 (1998) 177  
 Usami, A., Theoretical study of charge transportation in dye-sensitized nanocrystalline  $TiO_2$  electrodes 292 (1998) 223  
 Ushida, K., see Wang, Y. 299 (1999) 576  
 Usuba, S., see Katoh, R. 291 (1998) 305
- Vaara, J., J. Lounila and J. Jokisaari, Comment on "Nematic mixture methods for the determination of chemical shift anisotropy" 296 (1998) 541  
 Vaara, J., see Minaev, B. 295 (1998) 455  
 Vaara, J., see Ruud, K. 297 (1998) 467  
 Vaccaro, P.H., see Müller, T. 292 (1998) 243  
 Vahtras, O., see Minaev, B. 295 (1998) 455  
 Vaida, V., see Phillips, J.A. 296 (1998) 377  
 Vakhtin, A.B. and K. Sugawara, Sequential attachment of hydrogen molecules to niobium cluster cations 299 (1999) 553  
 Vala, M., see Lapinski, L. 300 (1999) 195  
 Van Caillie, C. and R.D. Amos, Static and dynamic polarisabilities, Cauchy coefficients and their anisotropies: a comparison of standard methods 291 (1998) 71  
 Vandaele, A.C., see Bernath, P. 297 (1998) 293  
 Van der Auweraer, M., see Latterini, L. 295 (1998) 11  
 Van der Auweraer, M., see Rommens, J. 294 (1998) 434  
 Van der Auweraer, M., see Scheblykin, I.G. 298 (1998) 341  
 Van der Heide, P.A.W. and J.W. Rabalais, Photoelectron spectroscopic study of the temperature-dependent termination of the  $LaAlO_3(100)$  surface 297 (1998) 350  
 Van der Veken, B.J., see Herrebout, W.A. 295 (1998) 223  
 Van Deun, R., see Binnemans, K. 300 (1999) 509  
 Van Faassen, E.E., see Kerp, H.R. 298 (1998) 302  
 Van Haesendonck, C., see Ahlskog, M. 300 (1999) 202  
 Van Leuken, J.J., see de Lange, M.J.L. 294 (1998) 332  
 Vannikov, A.V., see Tameev, A.R. 294 (1998) 605  
 Van Oijen, A.M., J. Köhler, J. Schmidt, M. Müller and G.J. Brakenhoff, 3-Dimensional super-resolution by spectrally selective imaging 292 (1998) 183

- Van Oosten, A.B. and F. Mila, Ab initio determination of exchange integrals and Néel temperature in the chain cuprates 295 (1998) 359
- Van Roij, A.J.A., see von Helden, G. 299 (1999) 171
- Van Zee, R.J. and W. Weltner Jr., ESR of the  $P_3^-$  radical: establishment of the electronic ground state 300 (1999) 243
- Varandas, A.J.C. and H. Szichman, A three-dimensional quantum mechanical study of the  $O + HO_2$  atmospheric reaction: infinite-order sudden approximation and novel adiabatic approaches vs. quasiclassical trajectories 295 (1998) 113
- Varandas, A.J.C. and P.E. Abreu, Quasi-ab initio dynamics: a test trajectory study of the  $H + H_2$  reaction using energies and gradients based on scaling of the external correlation 293 (1998) 261
- Varandas, A.J.C., S.P.J. Rodrigues and P.A.J. Gomes, Energy switching potential energy surfaces and spectra of the van der Waals modes for the ArHCN molecule 297 (1998) 458
- Varnavsky, O.P., see Scheblykin, I.G. 298 (1998) 341
- Vaughan, D.J., see Wright, K. 299 (1999) 527
- Vaval, N. and S. Pal, Molecular property calculations for excited states using a multireference coupled-cluster approach 300 (1999) 125
- Vaval, N., see Basu Kumar, A. 295 (1998) 189
- Vdovin, A., J. Sepiół, J. Jasny, J.M. Kauffman and A. Mordziński, Excited state proton transfer in jet-cooled 2,5-di-(2-benzoxazoly)phenol 296 (1998) 557
- Vdovin, A., see Sepiół, J. 296 (1998) 549
- Veber, M., see Lampre, I. 293 (1998) 423
- Vecchiocattivi, F., see Brunetti, B. 294 (1998) 584
- Vecer, J., see Konopasek, I. 293 (1998) 429
- Veciana, J., see García-Muñoz, J.L. 293 (1998) 160
- Vener, M.V. and S. Iwata, Model study of H-bonded  $ROH \dots (NH_3)_5$  clusters: a search for possible ground-state proton transfer species 292 (1998) 87
- Venkatnathan, A. and M.K. Mishra, The  $^2\Pi_g$  shape resonance in electron-acetylene scattering: an investigation using the dilated electron propagator method 296 (1998) 223
- Venkatraman, R., see Jabalameli, A. 295 (1998) 135
- Venugopal Rao, S., D. Narayana Rao, J.A. Akkara, B.S. DeCristofano and D.V.G.L.N. Rao, Dispersion studies of non-linear absorption in  $C_{60}$  using Z-scan 297 (1998) 491
- Veracini, C.A., see Calucci, L. 296 (1998) 357
- Verdasco, E., see Aoiz, F.J. 299 (1999) 25
- Verhagen, R., see Kentgens, A.P.M. 300 (1999) 435
- Verma, A.L., see Singh, R.K. 296 (1998) 611
- Vetere, V., see Arnaud, R. 293 (1998) 295
- Viant, M.R., see Cruzan, J.D. 292 (1998) 667
- Viappiani, C., see Murgida, D.H. 294 (1998) 538
- Vidović, D., see Gutman, I. 297 (1998) 428
- Vigliotti, F. and M. Chergui, Lineshape analysis of impurity Rydberg transitions in van der Waals solids: derivation of intermolecular potentials 296 (1998) 316
- Vikhrenko, V.S., see Heidelberg, C. 291 (1998) 333
- Vilchiz, V.H., see Klopfer, J.A. 298 (1998) 120
- Vilkas, M.J., K. Koc and Y. Ishikawa, Relativistic multireference Møller–Plesset perturbation theory based on multiconfigurational Dirac–Fock reference functions 296 (1998) 68
- Viñas, M.H., see García-Ochoa, I. 296 (1998) 335
- Vincent, M.A., see Wright, K. 299 (1999) 527

- Vittadini, A., see Casarin, M. 300 (1999) 403
- Vitukhnovsky, A.G., see Scheblykin, I.G. 298 (1998) 341
- Vivekanandan, S., see Khetrpal, C.L. 296 (1998) 537
- V. Kopylow, A. and D. Kolb, Accurate finite-element multi-grid (FEM-MG) description for angular momentum and spin dependences of Kohn-Sham density functionals for axially restricted calculations on first-row atoms and dimers 295 (1998) 439
- Vogel, E., see Sepiol, J. 296 (1998) 549
- Vogel, E., see Shuali, Z. 300 (1999) 687
- Voityuk, A.A., M.-E. Michel-Beyerle and N. Rösch, Structure and rotation barriers for ground and excited states of the isolated chromophore of the green fluorescent protein 296 (1998) 269
- Volk, M., see Metzler, R. 293 (1998) 477
- Völker, S., see den Hartog, F.T.H. 297 (1998) 314
- Volkmer, A., K. Wynne and D.J.S. Birch, Near-infrared excitation of alkane ultra-violet fluorescence 299 (1999) 395
- Voll, S., see Simon, M. 296 (1998) 579
- Volpp, H.-R., see Härle, H. 293 (1998) 26
- Von Helden, G., I. Holleman, M. Putter, A.J.A. van Roij and G. Meijer, Infrared resonance enhanced multi-photon ionization spectroscopy of  $C_{84}$  299 (1999) 171
- Voth, G.A., see Pavese, M. 300 (1999) 93
- Vullers, R.J.M., see Ahlskog, M. 300 (1999) 202
- Waclawik, E.R., A.C. Legon and J.H. Holloway, Rotational spectrum of the nitrogen trifluoride-chlorine monofluoride complex and the inductive effect of groups  $R = CH_3$ , H, F on  $R_3N/ClF$  interactions 295 (1998) 289
- Wada, M., see Houjou, H. 294 (1998) 162
- Wada, N., see Jamali, J.B. 292 (1998) 661
- Wadi, H. and L. Wiesenfeld, A fully geometrical analysis of indirect reactive scattering 300 (1999) 37
- Wahlgren, U., see Malkina, O.L. 296 (1998) 93
- Wakabayashi, T., see Takahashi, H. 294 (1998) 95
- Wales, D.J., Erratum to "Symmetry, near-symmetry and energetics" [Chem. Phys. Lett. 285 (1998) 330] 294 (1998) 262
- Walker, N.R., S. Firth and A.J. Stace, Stable Cu(II) co-ordination complexes in the gas phase 292 (1998) 125
- Wall, M.R., T. Dieckmann, J. Feigon and D. Neuhauser, Two-dimensional filter-diagonalization: spectral inversion of 2D NMR time-correlation signals including degeneracies 291 (1998) 465
- Wallenberg, L.R., see Suenaga, K. 300 (1999) 695
- Walters, J.K., N.T. Skipper and A.K. Soper, The interlayer structure of a graphite-potassium-ammonia intercalation compound by neutron diffraction 300 (1999) 444
- Walther, C., see Rousseau, R. 295 (1998) 41
- Waluk, J., see Møller, S. 291 (1998) 51
- Waluk, J., see Sepiol, J. 296 (1998) 549
- Wan, C.Z., see Yu, H.Z. 293 (1998) 1
- Wang, B., H. Hou and Y. Gu, Features of the potential energy surface for the decomposition of  $CH_3OF$  300 (1999) 99
- Wang, C., see Zhou, S. 297 (1998) 77
- Wang, C.-R., K.K.-W. Lo, W.K.-M. Fung and V.W.-W. Yam, Molecular orbital studies of luminescent tetranuclear copper(I) complexes 296 (1998) 505
- Wang, C.-R., M. Inakuma and H. Shinohara, Metallofullerenes  $Sc_2@C_{82}(I, II)$  and  $Sc_2@C_{86}(I, II)$ : isolation and spectroscopic studies 300 (1999) 379



- Wang, C.Z., see Pan, B.C. 292 (1998) 75
- Wang, D., see Cao, X. 299 (1999) 322
- Wang, E.G., see Yu, J. 292 (1998) 531
- Wang, G., see Pan, Z.W. 299 (1999) 97
- Wang, G.-J., see Zhang, H. 300 (1999) 483
- Wang, J. and L. Holmlid, Planar clusters of Rydberg matter  $K_N$  ( $N = 7, 14, 19, 37, 61$ ) detected by multiphoton fragmentation time-of-flight mass spectrometry 295 (1998) 500
- Wang, J.-K., see Tsai, C.-S. 295 (1998) 509
- Wang, N., Y.H. Tang, Y.F. Zhang, C.S. Lee, I. Bello and S.T. Lee, Si nanowires grown from silicon oxide 299 (1999) 237
- Wang, N., see Lu, X. 300 (1999) 109
- Wang, N., see Lü, X. 291 (1998) 445
- Wang, N.Q., see Xu, X. 292 (1998) 282
- Wang, P., M. Shiotani and S. Lunell, Structure and dynamics of radical cations of selectively deuteriated cyclohexanes: an ESR and ab initio study 292 (1998) 110
- Wang, P., see Wei, X. 300 (1999) 385
- Wang, S., see O'Keeffe, P. 298 (1998) 368
- Wang, S., see Zhang, T. 298 (1998) 236
- Wang, W., see Schenker, S. 297 (1998) 281
- Wang, X., H. Dang, Z. Gu and Q. Qin, A new hypermetallic molecule LaOMn generated by laser ablation 300 (1999) 739
- Wang, X., see Li, L. 291 (1998) 179
- Wang, Y., K. Ushida, Y. Tominaga and A. Kira, Molecular dynamics of acetophenone and its derivatives investigated by femtosecond optical Kerr effect spectroscopy and depolarized low-frequency Raman scattering 299 (1999) 576
- Wang, Y., see Liu, Y. 298 (1998) 315
- Wang, Y.A., see Govind, N. 295 (1998) 129
- Wang, Z.-X. and M.-B. Huang, Insertion of methylidyne into the C-H bond of ethylene 291 (1998) 381
- Warda, S.A., see Hu, Z. 297 (1998) 321
- Warman, J.M., see Scholes, G.D. 292 (1998) 601
- Warren, W.S., see Ahn, S. 291 (1998) 121
- Washida, N., see Yamaguchi, M. 298 (1998) 93
- Watanabe, O., see Fukazawa, H. 294 (1998) 554
- Watson, P.R., see Gannon, T.J. 300 (1999) 163
- Weber, J., see De Angelis, F. 291 (1998) 57
- Weber, S.E., B.V. Reddy, B.K. Rao and P. Jena, Chemically induced changes in the magnetic moments in transition metal monomers and dimers 295 (1998) 175
- Wee, A.T.S., T.W. Fishlock, R.A. Dixon, J.S. Foord, R.G. Egdell and J.B. Pethica, Bromine etching of mesoscopic structures on Cu(210): a scanning tunneling microscopy study 298 (1998) 146
- Weghorn, S.J., see Shuali, Z. 300 (1999) 687
- Wei, C.-Y., see Chou, P.-T. 294 (1998) 579
- Wei, C.-Y., see Chou, P.-T. 299 (1999) 327
- Wei, G.W., Quasi wavelets and quasi interpolating wavelets 296 (1998) 215
- Wei, X., C. Hu, Z. Suo, P. Wang, W. Zhang, Z. Xu and E.C. Alyea, Solid state  $^{13}\text{C}$  NMR and optical non-linearities study of  $\text{C}_{60}$  trimethylenediamine adducts 300 (1999) 385
- Weichert, A., see Riehn, C. 299 (1999) 103

- Weigend, F., M. Häser, H. Patzelt and R. Ahlrichs, RI-MP2: optimized auxiliary basis sets and demonstration of efficiency 294 (1998) 143
- Weiß, J., see Hauschildt, J. 300 (1999) 569
- Weis, P., see Kemper, P.R. 293 (1998) 503
- Weiser, P.S., D.A. Wild and E.J. Bieske, Infrared spectra of  $I^-(C_2H_2)_n$  ( $1 \leq n \leq 4$ ) anion complexes 299 (1999) 303
- Weisman, R.B., see Samuels, D.A. 295 (1998) 105
- Welling, L.L., see Gopinath, C.S. 296 (1998) 566
- Wells, L., see Yuan, J. 297 (1998) 553
- Weltner Jr., W., see Van Zee, R.J. 300 (1999) 243
- Wennmalm, S., see Edman, L. 292 (1998) 15
- Wennmalm, S., see Edman, L. 294 (1998) 625
- Wenthold, P.G., A computational study of the electron affinity of silene 297 (1998) 445
- Werncke, W., see Pfeiffer, M. 295 (1998) 56
- Werst, D.W., see Chemerisov, S.D. 291 (1998) 262
- Weschke, E., see Meier, R. 292 (1998) 507
- Westcott, S.L., S.J. Oldenburg, T.R. Lee and N.J. Halas, Construction of simple gold nanoparticle aggregates with controlled plasmon-plasmon interactions 300 (1999) 651
- Wetterauer, U., A. Pusel and P. Hess, VUV photodesorption of molecular hydrogen from the hydrogenated silicon(111) surface 300 (1999) 397
- Wheatley, R.J., An overlap model for exchange-induction: application to alkali halides 294 (1998) 487
- White, M.G., see Wiedmann, R.T. 293 (1998) 391
- Wiberg, K.B., R.E. Stratmann and M.J. Frisch, A time-dependent density functional theory study of the electronically excited states of formaldehyde, acetaldehyde and acetone 297 (1998) 60
- Wiedmann, R.T., L. Goodman and M.G. White, Two-color zero kinetic energy-pulsed field ionization spectroscopy of the acetone  $n$ -radical cation: the  $a_2$  torsional vibration 293 (1998) 391
- Wiesen, P., see Becker, K.H. 300 (1999) 460
- Wiesenfeld, L., see Wadi, H. 300 (1999) 37
- Wight, C.A., see Misochko, E.Ya. 293 (1998) 547
- Wild, D.A., see Weiser, P.S. 299 (1999) 303
- Wilhelm, T., see Wurzer, A.J. 299 (1999) 296
- Willetts, A., see Skylaris, C.-K. 296 (1998) 445
- Williams, J.S., see Chen, Y. 299 (1999) 260
- Willms, L., see Härle, H. 293 (1998) 26
- Wilson, G.L., see Moog, R.S. 299 (1999) 265
- Wincel, H., Gas-phase clustering reactions of  $NO^+$  and  $NO_2^+$  with  $CH_3NO_2$  292 (1998) 193
- Wind, P., see Miguel, B. 294 (1998) 49
- Winkler, B. and V. Milman, Structure and properties of supercubane from density functional calculations 293 (1998) 284
- Winnewisser, G., see Linnartz, H. 292 (1998) 188
- Winnewisser, G., see Roth, D.A. 298 (1998) 381
- Winnewisser, M., see Koput, J. 295 (1998) 462
- Witte, G., see Senet, P. 299 (1999) 389
- Wittig, C., see Liu, K. 299 (1999) 374
- Wolber, J., S.J. Doran, M.O. Leach and A. Bifone, Measuring diffusion of xenon in solution with hyperpolarized  $^{129}Xe$  NMR 296 (1998) 391
- Wolf, M., see Bartels, L. 291 (1998) 573
- Wolfrum, J., see Härle, H. 293 (1998) 26

- Wolfrum, J., see Schäfer, J. 300 (1999) 152
- Wolfrum, J., see Schneider-Kühnle, Y. 294 (1998) 191
- Wolfsberg, M., see Fritzsche, S. 296 (1998) 253
- Woliński, P., see Olszewski, R. 297 (1998) 537
- Wöll, C., see Bagus, P.S. 294 (1998) 599
- Wong, M.W., see Flammang, R. 300 (1999) 183
- Workman, M.A. and J.S. Francisco, Molecular structure and energetics of  $\text{BrO}_x$  radicals (where  $x = 1, 2$ , and  $3$ ) 293 (1998) 65
- Worth, G.A., H.-D. Meyer and L.S. Cederbaum, State filtering by a bath: up to 24 mode numerically exact wavepacket propagations 299 (1999) 451
- Wright, D., see Grunnet-Jepsen, A. 291 (1998) 553
- Wright, J.S., see DiLabio, G.A. 297 (1998) 181
- Wright, K., I.H. Hillier, D.J. Vaughan and M.A. Vincent, Cluster models of the dissociation of water on the surface of galena (PbS) 299 (1999) 527
- Wright, T.G., see Lee, E.P.F. 295 (1998) 354
- Wu, C. and E.D. Poliakoff, Vibrationally resolved  $2a_{2u}^{-1}$  photoionization of  $\text{C}_6\text{F}_6$  292 (1998) 167
- Wu, G., Classification and assignment of eigenstates of highly excited vibrational manifolds via broken constants of motion 292 (1998) 369
- Wu, G., Zinc-67 nuclear magnetic resonance spectroscopy of solids 298 (1998) 375
- Wu, W., S. Zhong and S. Shaik, VBDFT(s): a Hückel-type semi-empirical valence bond method scaled to density functional energies. Application to linear polyenes 292 (1998) 7
- Wurzer, A.J., T. Wilhelm, J. Piel and E. Riedle, Comprehensive measurement of the  $\text{S}_1$  azulene relaxation dynamics and observation of vibrational wavepacket motion 299 (1999) 296
- Wyatt, R.E., see Minehardt, T.J. 295 (1998) 373
- Wynne, K., see Volkmer, A. 299 (1999) 395
- Xagas, A., see Provata, A. 297 (1998) 484
- Xantheas, S.S., see Froudakis, G.E. 294 (1998) 109
- Xantheas, S.S., see Müller, T. 293 (1998) 72
- Xia, S., see Zhang, W. 292 (1998) 133
- Xiao, M., see Cruz, D.A. 297 (1998) 225
- Xie, P., see Zhang, W. 292 (1998) 133
- Xie, S.S., see Pan, Z.W. 299 (1999) 97
- Xu, C., see Taylor, T.R. 297 (1998) 133
- Xu, G., see Yu, J. 292 (1998) 531
- Xu, G., see Zhang, T. 298 (1998) 236
- Xu, K., see Zhang, J. 299 (1999) 285
- Xu, X., H. Nakatsuji, M. Ehara, X. Lü, N.Q. Wang and Q.E. Zhang, Cluster modeling of metal oxides: the influence of the surrounding point charges on the embedded cluster 292 (1998) 282
- Xu, X., see Lu, X. 300 (1999) 109
- Xu, X., see Lü, X. 291 (1998) 445
- Xu, Y., see Zhou, S. 297 (1998) 77
- Xu, Z., see Wei, X. 300 (1999) 385
- Xu, Z.-F., see Yu, Y.-X. 296 (1998) 131
- Xue, D. and S. Zhang, Linear and nonlinear optical properties of  $\text{KNbO}_3$  291 (1998) 401
- Yagi, M., see Noda, M. 296 (1998) 599
- Yagishita, A., see Adachi, J. 294 (1998) 559



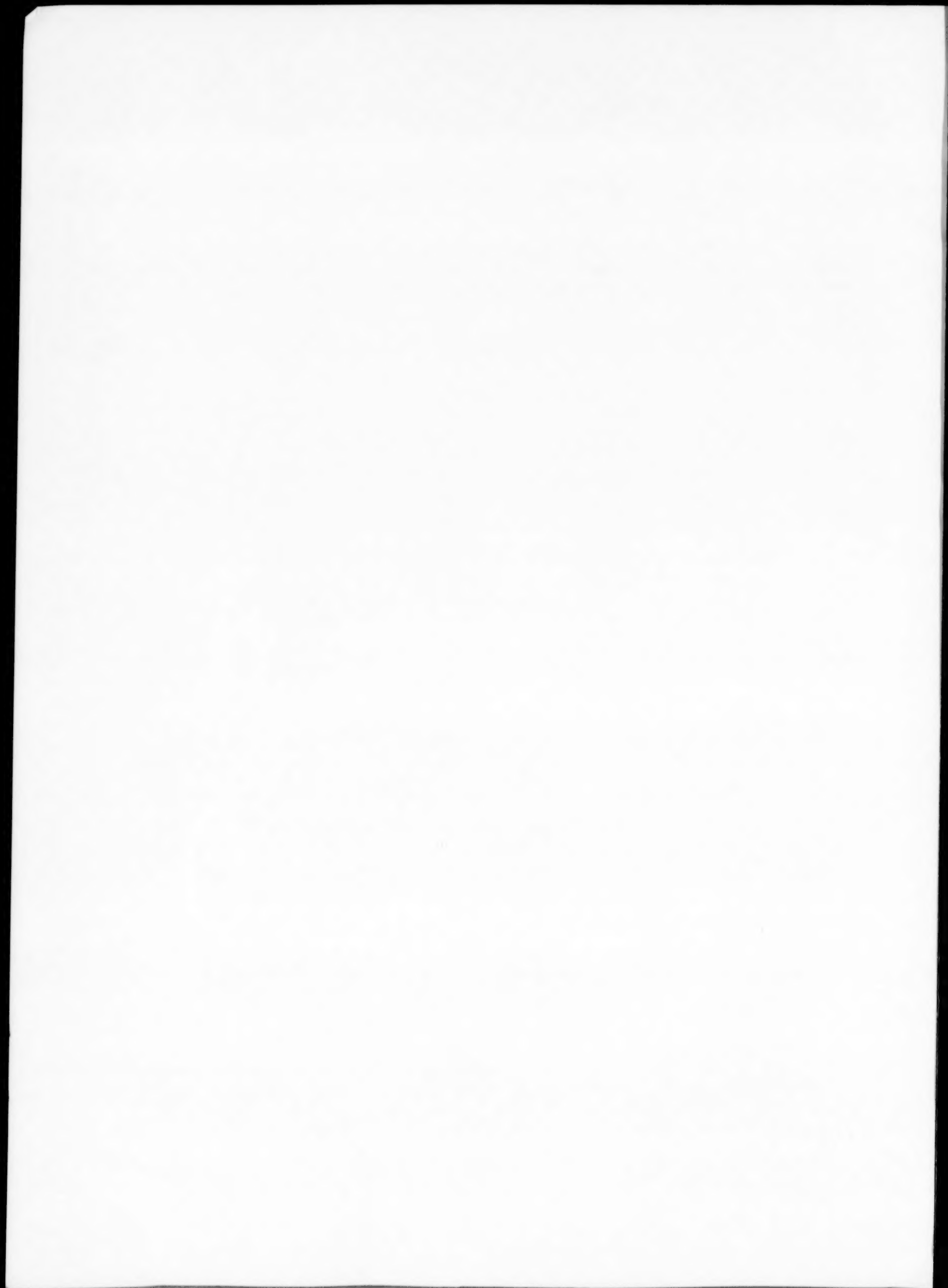
- Yakovlev, V.A., see Alieva, E.V. 292 (1998) 542
- Yam, V.W.-W., see Wang, C.-R. 296 (1998) 505
- Yamabe, S., see Hiraoka, K. 299 (1999) 545
- Yamaguchi, K., see Nakano, M. 295 (1998) 317
- Yamaguchi, K., see Nakano, M. 295 (1998) 328
- Yamaguchi, K., see Nishino, M. 297 (1998) 51
- Yamaguchi, K., see Yoshioka, Y. 294 (1998) 459
- Yamaguchi, M., M. Furubayashi, S. Inomata and N. Washida, Analysis of laser-induced fluorescence spectra of the  $\tilde{B}(^2A'')-\tilde{X}(^2A'')$  transition with calculated Franck-Condon factors of  $\text{CH}_2\text{CFO}$  298 (1998) 93
- Yamaguchi, T., see Nishino, Y. 296 (1998) 408
- Yamaguchi, Y., J.C. Rienstra-Kiracofe, J.C. Stephens and H.F. Schaefer III, The hydroxyethynyl radical (CCOH): an accessible isomer of the ketenyl radical (HCCO)? 291 (1998) 509
- Yamamoto, N., see Ohtani, H. 299 (1999) 571
- Yamane, T., Y. Inoue and M. Sakurai, A new simulated annealing method combined with a polarizable continuum model based on the boundary element method 291 (1998) 137
- Yamanouchi, K., see Hashimoto, N. 291 (1998) 130
- Yamanouchi, K., see Sako, T. 294 (1998) 571
- Yamanouchi, K., see Sako, T. 299 (1999) 35
- Yamaoka, H., H. Matsuoka, K. Kago, H. Endo, J. Eckelt and R. Yoshitome, Monolayer X-ray reflectometry at the air-water interface 295 (1998) 245
- Yamataka, H., M. Aida and M. Dupuis, One transition state leading to two product states: ab initio molecular dynamics simulations of the reaction of formaldehyde radical anion and methyl chloride 300 (1999) 583
- Yamataka, H., see Aida, M. 292 (1998) 474
- Yamauchi, S., see Fujisawa, J. 294 (1998) 248
- Yamazaki, I., see Ohta, N. 292 (1998) 535
- Yamazaki, T., Y. Aoki and A. Imamura, A method for calculating electric dipole transition moments using small configuration interaction spaces based on the concept of interaction frontier orbitals 295 (1998) 431
- Yan, K., see Zhang, W. 292 (1998) 133
- Yan, W., see Zhang, T. 298 (1998) 236
- Yan, Y.J., see He, R.R. 298 (1998) 170
- Yanagi, H., T. Hishiki, T. Tobitani, A. Otomo and S. Mashiko, Thin film lasing from a dye-doped silica/titania composite 292 (1998) 332
- Yang, H., see Zhang, T. 298 (1998) 236
- Yang, J.-P., see Paa, W. 292 (1998) 607
- Yang, X. and P.J. Dagdigan, Selective rotational energy transfer from individual  $\Lambda$ -doublet levels of highly rotationally excited  $\text{CN}(A^2\Pi)$  297 (1998) 506
- Yang, Z.-Z. and D.-X. Zhao, A characteristic molecular contour evaluated by a theoretical method 292 (1998) 387
- Yano, S., see Nishino, Y. 296 (1998) 408
- Yaseen, M., see Baig, M.A. 296 (1998) 403
- Ye, C.-H., see Ren, H.-L. 292 (1998) 317
- Yee-Madeira, H., see Aquino, N. 296 (1998) 111
- Yersin, H., see Strasser, J. 295 (1998) 95
- Yi, Z., see Micha, D.A. 298 (1998) 250
- Yildirim, T., see Guerrero, H.M. 297 (1998) 265

- Yin, M., see Zhang, W. 292 (1998) 133
- Yokoi, H., see Katoh, R. 291 (1998) 305
- Yokojima, S. and G.H. Chen, Linear-scaling localized-density-matrix method for the ground and excited states of one-dimensional molecular systems 300 (1999) 540
- Yokojima, S. and G.H. Chen, Time domain localized-density-matrix method 292 (1998) 379
- Yokoyama, T., see Terada, S. 300 (1999) 645
- Yonemitsu, K., see Imamura, Y. 298 (1998) 15
- Yonezawa, Y., see Kometani, N. 294 (1998) 619
- Yoon, M.-C., Y.S. Choi and S.K. Kim, The OH production from the  $\pi-\pi^*$  transition of acetylacetone 300 (1999) 207
- Yoshida, Y., Y. Kubozono, S. Kashino and Y. Murakami, Structure and electronic properties of  $\text{Cs}_3\text{C}_{60}$  under ambient pressure revealed by X-ray diffraction and ESR 291 (1998) 31
- Yoshikawa, H., K. Sasaki and H. Masuhara, Picosecond fluorescence analysis of charge transfer microcrystals by near-field microspectroscopy 293 (1998) 185
- Yoshimori, A., see Jigato, M.P. 300 (1999) 639
- Yoshioka, N., see Tsuchimoto, M. 297 (1998) 115
- Yoshioka, Y., S. Kubo, K. Yamaguchi and I. Saito, An ab initio molecular orbital study of a binuclear dioxygen complex as a model of the binuclear active site in cytochrome *c* oxidase 294 (1998) 459
- Yoshioka, Y., see Nishino, M. 297 (1998) 51
- Yoshitome, R., see Yamaoka, H. 295 (1998) 245
- Yu, H.-G. and G. Nyman, A spectral transform Krylov subspace iteration approach to quantum scattering 298 (1998) 27
- Yu, H.Z., J.S. Baskin, B. Steiger, C.Z. Wan, F.C. Anson and A.H. Zewail, Femtosecond dynamics of metalloporphyrins: electron transfer and energy redistribution 293 (1998) 1
- Yu, J., E.G. Wang and G. Xu, Observations of micrometer BCN rods by bias-assisted hot-filament chemical vapor deposition 292 (1998) 531
- Yu, W.-S., see Chou, P.-T. 299 (1999) 327
- Yu, Y.-X., S.-M. Li, Z.-F. Xu, Z.-S. Li and C.-C. Sun, An ab initio study on the reaction  $\text{NH}_2 + \text{CH}_4 \rightarrow \text{NH}_3 + \text{CH}_3$  296 (1998) 131
- Yuan, J., L. Wells and P. Marshall, Kinetic studies of the reaction of atomic hydrogen with trifluoroiodomethane 297 (1998) 553
- Yudasaka, M., T. Ichihashi, T. Komatsu and S. Iijima, Single-wall carbon nanotubes formed by a single laser-beam pulse 299 (1999) 91
- Yue, Y., see Ren, H.-L. 292 (1998) 317
- Zacharias, H., see Rudert, A.D. 294 (1998) 381
- Zagrodzki, B., see Borowicz, P. 291 (1998) 351
- Zaitsev, N.N., see Osad'ko, I.S. 293 (1998) 138
- Zajac, A., see Svrček, M. 299 (1999) 151
- Zannoni, C., see Berardi, R. 297 (1998) 8
- Zannoni, C., see Stelzer, J. 299 (1999) 9
- Zehnacker, A., F. Lahmani, J.P. Desvergne and H. Bouas-Laurent, Conformation-dependent intramolecular exciplex formation in jet-cooled bichromophores 293 (1998) 357
- Zeiri, Y., G. Katz, R. Kosloff, M.S. Topaler, D.G. Truhlar and J.C. Polanyi, Quantum mechanism in the photodissociation of NaFH complex: a challenge to semiclassical analysis 300 (1999) 523
- Zenkevich, E., see Knyukshto, V. 297 (1998) 97

- Zentz, C., see Haouz, A. 294 (1998) 197
- Zerbetto, F., see Fowler, P.W. 300 (1999) 369
- Zerner, M.C., see Reinot, T. 299 (1999) 410
- Zerza, G., see Portella-Oberli, M.T. 296 (1998) 323
- Zewail, A.H., see Chachisvilis, M. 293 (1998) 153
- Zewail, A.H., see Møller, K.B. 295 (1998) 1
- Zewail, A.H., see Møller, K.B. 296 (1998) 619
- Zewail, A.H., see Yu, H.Z. 293 (1998) 1
- Zewail, A.H., see Zhong, D. 298 (1998) 129
- Zhabotinsky, A.M., see Kurin-Csörgei, K. 295 (1998) 70
- Zhan, L.X., see Zhang, Y.C. 300 (1999) 27
- Zhang, B.-J., An improvement of the macroscopic compressibility approximation 296 (1998) 266
- Zhang, D.H., see Zhu, W. 292 (1998) 46
- Zhang, F.,  $2\pi$ -Twistons in crystalline polyethylene 293 (1998) 499
- Zhang, F.S., E. Suraud, F. Calvo and F. Spiegelmann, Vibrational properties of sodium microclusters 300 (1999) 595
- Zhang, H., R. Zhu, G.-J. Wang, K.-L. Han, G.-Z. He and N.-Q. Lou, Photofragment translational spectroscopy of *p*-bromotoluene at 266 nm 300 (1999) 483
- Zhang, J., K. Xu and G. Amaral, Ultraviolet photodissociation dynamics of  $\text{HN}_3$ : the  $\text{H} + \text{N}_3$  channel 299 (1999) 285
- Zhang, J.-P., see Satishkumar, B.C. 300 (1999) 473
- Zhang, J.-X. and P.M. Aker, Charge-enhanced uptake of  $\text{SO}_2$  at the water/air interface 298 (1998) 183
- Zhang, J.Z.H., see Ge, J.-Y. 292 (1998) 51
- Zhang, J.Z.H., see Zhang, Y.C. 300 (1999) 27
- Zhang, J.Z.H., see Zhu, W. 292 (1998) 46
- Zhang, Q., see Lu, X. 300 (1999) 109
- Zhang, Q., see Lü, X. 291 (1998) 445
- Zhang, Q.E., see Xu, X. 292 (1998) 282
- Zhang, Q.G., see Zhang, Y.C. 300 (1999) 27
- Zhang, S., see Xue, D. 291 (1998) 401
- Zhang, T., C. Chen, Q. Gong, W. Yan, S. Wang, H. Yang, H. Jian and G. Xu, Time-resolved excited state dynamics of a cyanine dye 298 (1998) 236
- Zhang, W., P. Xie, C. Duan, K. Yan, M. Yin, L. Lou, S. Xia and J.-C. Krupa, Preparation and size effect on concentration quenching of nanocrystalline  $\text{Y}_2\text{SiO}_5\text{:Eu}$  292 (1998) 133
- Zhang, W., see Wei, X. 300 (1999) 385
- Zhang, W.X., see Pang, W.N. 299 (1999) 207
- Zhang, Y.C., L.X. Zhan, Q.G. Zhang, W. Zhu and J.Z.H. Zhang, Quantum wavepacket calculation for the ion molecule reaction  $\text{N}^+ + \text{H}_2 \rightarrow \text{NH}^+ + \text{H}$  300 (1999) 27
- Zhang, Y.F., see Wang, N. 299 (1999) 237
- Zhao, C., see Polavarapu, P.L. 296 (1998) 105
- Zhao, D.-X., see Yang, Z.-Z. 292 (1998) 387
- Zheng, X. and D.L. Phillips, Examination of the A-band short-time photodissociation dynamics of the equatorial conformer of iodocyclohexane 296 (1998) 173
- Zheng, X., Y.F. Cheng and D.L. Phillips, A-band resonance Raman spectra of 1,2-diiodoethane in cyclohexane solution. Substituent effects on the 1-halo-2-iodoethane short-time photodissociation dynamics 292 (1998) 295
- Zheng, Y., see Pang, W.N. 299 (1999) 207
- Zheng, Y.-J., see Lam, A.M. 292 (1998) 229



- Zhong, D., E.W.-G. Diau, T.M. Bernhardt, S. De Feyter, J.D. Roberts and A.H. Zewail, Femtosecond dynamics of valence-bond isomers of azines: transition states and conical intersections 298 (1998) 129
- Zhong, S., see Wu, W. 292 (1998) 7
- Zhou, S., Y. Liu, Y. Xu, W. Hu, D. Zhu, X. Qiu, C. Wang and C. Bai, Rectifying behaviors of Langmuir-Blodgett films of an asymmetrically substituted phthalocyanine 297 (1998) 77
- Zhou, W. and J. Klinowski, The mechanism of channel formation in the mesoporous molecular sieve MCM-41 292 (1998) 207
- Zhou, W.Y., see Pan, Z.W. 299 (1999) 97
- Zhu, C., see Mil'nikov, G.V. 293 (1998) 448
- Zhu, D., see Fan, L. 294 (1998) 443
- Zhu, D., see Zhou, S. 297 (1998) 77
- Zhu, J., see He, R.R. 298 (1998) 170
- Zhu, L., see Tsukuda, T. 295 (1998) 416
- Zhu, R., see Zhang, H. 300 (1999) 483
- Zhu, W., J.Z.H. Zhang and D.H. Zhang, Full-dimensional quantum dynamics calculation for  $D_2 + CN$  reaction 292 (1998) 46
- Zhu, W., see Zhang, Y.C. 300 (1999) 27
- Zicovich-Wilson, C.M., see Civalleri, B. 292 (1998) 394
- Ziherl, P., R. Podgornik and S. Žumer, Casimir force in liquid crystals close to the nematic-isotropic phase transition 295 (1998) 99
- Zimmer, K., M. Hoppmeier and A. Schweig, Fluorescence of an organic radical cation (5,10-dihydro-5,10-dimethylphenazine<sup>•+</sup>) in liquid solution at room temperature 293 (1998) 366
- Zimmermann, M., see Riehn, C. 299 (1999) 103
- Zimmermann, T., see Häupl, T. 291 (1998) 215
- Zink, J.I., see Anderson, S.M. 291 (1998) 387
- Ziurys, L.M., see Allen, M.D. 293 (1998) 397
- Ziurys, L.M., see Apponi, A.J. 298 (1998) 161
- Zobov, N.F., see Császár, A.G. 293 (1998) 317
- Zubek, M., see Olszewski, R. 297 (1998) 537
- Zuckerman, D.M., see Fisher, M.E. 293 (1998) 461
- Žumer, S., see Ziherl, P. 295 (1998) 99
- Zúñiga, J., A. Bastida, M. Alacid and A. Requena, Optimal generalized internal vibrational coordinates for symmetrical linear triatomic molecules 298 (1998) 36



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